

(FILE 'HOME' ENTERED AT 12:41:45 ON 22 MAR 2006)

L1 FILE 'CAPLUS' ENTERED AT 12:41:55 ON 22 MAR 2006  
STRUCTURE UPLOADED  
S L1

L2 FILE 'REGISTRY' ENTERED AT 12:42:17 ON 22 MAR 2006  
0 S L1

L3 FILE 'CAPLUS' ENTERED AT 12:42:18 ON 22 MAR 2006  
0 S L2  
S L1

L4 FILE 'REGISTRY' ENTERED AT 12:42:26 ON 22 MAR 2006  
1 S L1 FULL

L5 FILE 'CAPLUS' ENTERED AT 12:42:27 ON 22 MAR 2006  
2 S L4 FULL

L6 FILE 'CAPLUS' ENTERED AT 12:45:04 ON 22 MAR 2006  
2 S 117528-59-3/PREP  
L7 0 S 117528-59-3/PROC  
L8 0 S 117528-59-3/PUR

L9 FILE 'CAPLUS' ENTERED AT 13:42:27 ON 22 MAR 2006  
STRUCTURE UPLOADED  
S L9

L10 FILE 'REGISTRY' ENTERED AT 13:42:49 ON 22 MAR 2006  
0 S L9

L11 FILE 'CAPLUS' ENTERED AT 13:42:49 ON 22 MAR 2006  
0 S L10  
S L9

L12 FILE 'REGISTRY' ENTERED AT 13:42:56 ON 22 MAR 2006  
1 S L9 FULL

L13 FILE 'CAPLUS' ENTERED AT 13:42:56 ON 22 MAR 2006  
3 S L12 FULL

FILE 'STNGUIDE' ENTERED AT 13:45:26 ON 22 MAR 2006

L14 FILE 'CAPLUS' ENTERED AT 13:51:46 ON 22 MAR 2006  
STRUCTURE UPLOADED  
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L15 FILE 'REGISTRY' ENTERED AT 13:52:09 ON 22 MAR 2006  
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L16 FILE 'CAPLUS' ENTERED AT 13:52:10 ON 22 MAR 2006  
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L17 FILE 'REGISTRY' ENTERED AT 13:52:15 ON 22 MAR 2006  
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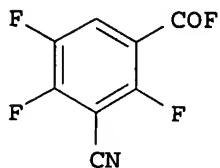
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4 S L17 FULL  
L19 4 S 195532-66-2/PREP  
L20 0 S 195532-66-2/PUR  
L21 0 S 195532-66-2/PROC  
L22 0 S L19 AND PY<1997

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DOCUMENT NUMBER: 129:316044  
 TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and intermediates for its production  
 INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
 PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
 SOURCE: PCT Int. Appl., 30 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
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JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
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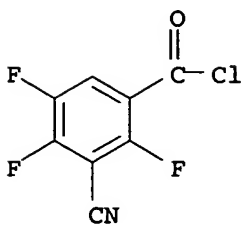
GI



AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

IT 195532-66-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 195532-66-2 CAPLUS



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

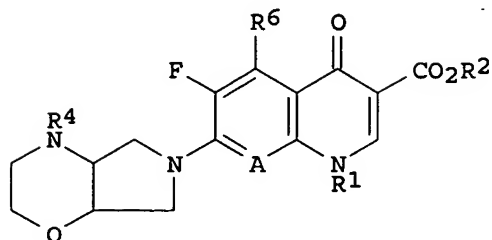
L18 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1998:406218 CAPLUS  
DOCUMENT NUMBER: 129:81719  
TITLE: Preparation of 7-(2-oxa-5,8-diazabicyclo[4.3.0]non-8-yl)quinolone- and -naphthyridonecarboxylic acid derivatives for therapy of Helicobacter pylori infections and associated gastroduodenal illnesses  
INVENTOR(S): Matzke, Michael; Petersen, Uwe; Jaetsch, Thomas; Bartel, Stephan; Schenke, Thomas; Himmeler, Thomas; Baasner, Bernd; Werling, Hans-Otto; Schaller, Klaus; Labischinski, Harald  
PATENT ASSIGNEE(S): Bayer A.-G., Germany  
SOURCE: Ger. Offen., 16 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19652239	A1	19980618	DE 1996-19652239	19961216
CA 2274894	AA	19980625	CA 1997-2274894	19971204
WO 9826779	A1	19980625	WO 1997-EP6781	19971204
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 717751	B2	20000330		
EP 946176	A1	19991006	EP 1997-954354	19971204
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BR 9714032	A	20000509	BR 1997-14032	19971204
JP 2000514825	T2	20001107	JP 1998-527250	19971204
JP 3463939	B2	20031105		
JP 2000351781	A2	20001219	JP 2000-154543	19971204
NZ 336228	A	20001222	NZ 1997-336228	19971204
AT 214929	E	20020415	AT 1997-954354	19971204
PT 946176	T	20020830	PT 1997-954354	19971204
ES 2175519	T3	20021116	ES 1997-954354	19971204
SK 283224	B6	20030304	SK 2000-1496	19971204
SK 283223	B6	20030304	SK 1999-795	19971204
EE 4090	B1	20030815	EE 1999-248	19971204
IL 130311	A1	20040104	IL 1997-130311	19971204
BG 64615	B1	20050930	BG 1999-103474	19990608
NO 9902903	A	19990614	NO 1999-2903	19990614

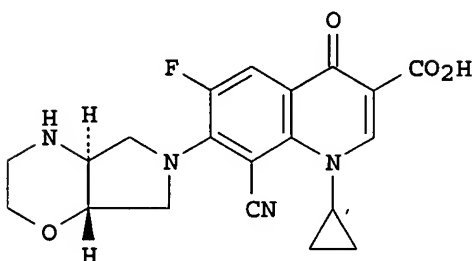
US 6133260	A	20001017	US 1999-319888	19990614
US 6432948	B1	20020813	US 1999-436316	19991108
NZ 506162	A	20010629	NZ 2000-506162	20000804

PRIORITY APPLN. INFO.:  
 DE 1996-19652239 A 19961216  
 JP 1998-527250 A3 19971204  
 NZ 1997-336228 A 19971204  
 WO 1997-EP6781 W 19971204  
 US 1999-319888 A3 19990614

OTHER SOURCE(S): MARPAT 129:81719  
 GI



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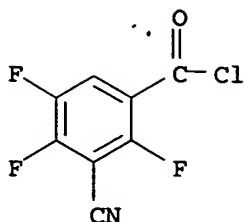


II

AB The title compds. [I; A = N, CR3; R1 = C1-4 (halo)alkyl; (fluoro)phenyl; (fluoro)cyclopropyl; R2 = H, (un)substituted C1-4 alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; R3 = H, halo, Me, MeO, CHF2O, cyano; R1R3 = OCH2CHMe or OCH2NMe bound to A via O atom; R4 = H, PhCH2, C1-3 alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl, CH:CHCO2R5, etc.; R5 = Me, Et; R6 = H, amino, OH, Me, halo], their racemates, diastereomer mixts., enantiomers, diastereoisomers and pharmaceutically acceptable hydrates and salts, were prepared For example, stirring 200 mg Et 8-cyano-1-cyclopropyl-6,7-difluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylate (7-step preparation from 3-bromo-2,4,5-trifluorobenzoyl fluoride given) with 97 mg (1S,6S)-2-oxa-5,8-diazabicyclo[4.3.0]nonane and 0.9 mL Et3N for 25 h at 40-45° in 30 mL MeCN under Ar, working up the product, saponifying by stirring with 30 mg LiOH·H2O in aqueous THF for 16 h at ambient temperature and acidifying the carboxylate salt with HCl gave 57% II-HCl (m. >300°). II at 2 + 10 mg/kg in H. pylori-infected mice gave after 7 days 100% clearing, vs. 0% for ciprofloxacin.

IT 195532-66-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and condensation with Et 3-dimethylaminoacrylate; preparation of (oxadiazabicyclononyl)quinolone- and -naphthyridonecarboxylic acid derivs. as drugs for therapy of Helicobacter pylori infections and associated gastroduodenal illnesses)

RN 195532-66-2 CAPLUS  
 CN Benzoyl chloride, 3-cyano-2,4,5-trifluoro- (9CI) (CA INDEX NAME)



L18 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:406214 CAPLUS

DOCUMENT NUMBER: 129:81718

TITLE: Use of 7-(1-aminomethyl-2-oxa-7-azabicyclo(3.3.0)oct-7-yl)-quinolonecarboxylates, -naphthyridonecarboxylates, and related compounds for Helicobacter pylori infection therapy and associated gastroduodenal illnesses.

INVENTOR(S): Petersen, Uwe; Matzke, Michael; Jaetsch, Thomas; Schenke, Thomas; Himmler, Thomas; Bartel, Stephan; Baasner, Bernd; Werling, Hans-Otto; Schaller, Klaus; Labischinski, Harald; Endermann, Rainer

PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 32 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

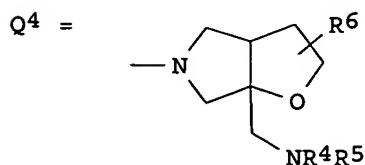
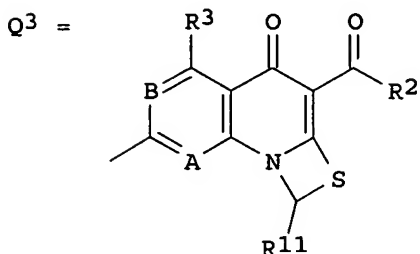
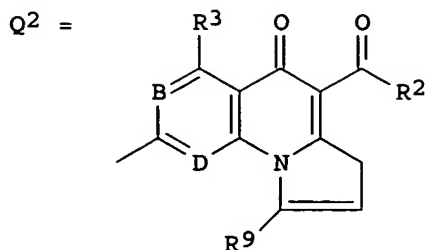
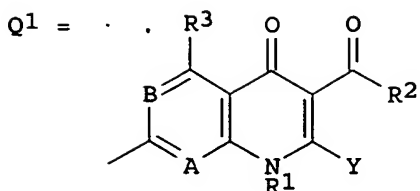
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19652219	A1	19980618	DE 1996-19652219	19961216
CA 2274892	AA	19980625	CA 1997-2274892	19971203
WO 9826768	A2	19980625	WO 1997-EP6751	19971203
WO 9826768	A3	19980806		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9858538	A1	19980715	AU 1998-58538	19971203
EP 944385	A2	19990929	EP 1997-954350	19971203
EP 944385	B1	20021016		
R: DE, ES, FR, GB, IT				
JP 2001506242	T2	20010515	JP 1998-527239	19971203
ES 2184150	T3	20030401	ES 1997-954350	19971203
US 6288081	B1	20010911	US 1999-319848	19990806
US 2001036941	A1	20011101	US 2001-829776	20010410
PRIORITY APPLN. INFO.:			DE 1996-19652219	A 19961216
			WO 1997-EP6751	W 19971203
			US 1999-319848	A3 19990806

OTHER SOURCE(S): MARPAT 129:81718

GI



AB Use of TQ [Q = Q1-Q3; T = Q4; A = N, CR7; B = N, CH, CF, CCl, CNO2, CNH2; D = N, CR10; Y = H; YR2 = SNH; R1 = (substituted) alkyl, alkenyl, cycloalkyl, bicyclo[1.1.1]pent-1-yl, 1,1-dimethylpropargyl, 3-oxetanyl, MeO, amino, etc.; R2 = OH, (substituted) alkoxy, PhCH2O, allyloxy, propargyloxy, acetoxymethoxy, etc.; R3 = H, amino, OH, Me, halo; R7 = H, halo, CF3, OMe, OCHF2, Me, cyano, CH:CH2, C.tplbond.CH; R1R7 = CH2CHMe, SCH2CH2, SCH2CHMe, etc.; R9 = H, (substituted) alkyl; R10 = H, halo, CF3, OMe, OCHF2, Me; R9R10 = OCH2, NHCH2, NMeCH2, SCH2, etc.; R11 = H, Me, CH2F; R4 = H, Me, Et, (substituted) acyl, alkoxycarbonyl, aminocarbonyl, etc.; R5 = H, Me, Et; R6 = H, Me], for treatment of Helicobacter pylori infection and associated gastroduodenal illnesses is claimed. Thus, 7-(1-aminomethyl-2-oxa-7-azobicyclo[3.3.0]oct-7-yl)-1-cyclopropyl-8-difluoromethoxy-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid (preparation given) had a min. inhibitory concentration of 0.006 mg/L against H. pylori 008.

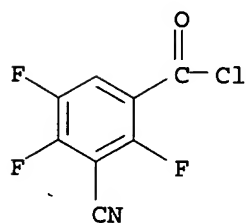
IT 195532-66-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

((aminomethyl)oxaazabicyclooctyl)quinolonecarboxylates, -naphthyridonecarboxylates, and related compds. for Helicobacter pylori infection therapy and associated gastroduodenal illnesses)

RN 195532-66-2 CAPLUS

CN Benzoyl chloride, 3-cyano-2,4,5-trifluoro- (9CI) (CA INDEX NAME)



L18 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:579724 CAPLUS

DOCUMENT NUMBER: 127:248093

TITLE: 8-Cyano-1-cyclopropyl-7-(2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid derivatives

INVENTOR(S): Bartel, Stefan; Jaetsch, Thomas; Himmeler, Thomas; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; Stegemann, Michael; Stupp, Hans-Peter; Wetzstein, Heinz-Georg

PATENT ASSIGNEE(S): Bayer A.-G., Germany; Bartel, Stefan; Jaetsch, Thomas;

Himmeler, Thomas; Rast, Hans-Georg; Hallenbach, Werner;  
Heinen, Ernst; Pirro, Franz; Scheer, Martin; et al.

SOURCE:

PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731001	A1	19970828	WO 1997-EP637	19970212
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RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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ZA 9701507	A	19970916	ZA 1997-1507	19970202
CA 2247020	AA	19970828	CA 1997-2247020	19970212
CA 2247020	C	20051108		
AU 9717689	A1	19970910	AU 1997-17689	19970212
AU 715341	B2	20000120		
EP 882049	A1	19981209	EP 1997-903260	19970212
EP 882049	B1	20021120		
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CN 1211984	A	19990324	CN 1997-192523	19970212
CN 1073112	B	20011017		
BR 9707606	A	19990727	BR 1997-7606	19970212
NZ 331468	A	20000228	NZ 1997-331468	19970212
JP 2000504734	T2	20000418	JP 1997-529755	19970212
IL 125444	A1	20010319	IL 1997-125444	19970212
RU 2173318	C2	20010910	RU 1998-117814	19970212
EP 1215202	A1	20020619	EP 2002-6519	19970212
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AT 228130	E	20021215	AT 1997-903260	19970212
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PT 882049	T	20030430	PT 1997-903260	19970212
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SK 284542	B6	20050602	SK 1998-1146	19970212
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NO 9803819	A	19980820	NO 1998-3819	19980820
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HK 1018903	A1	20020510	HK 1999-104030	19990917
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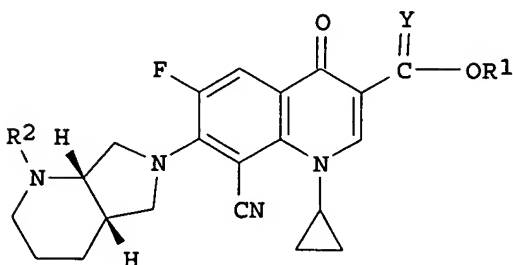
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WO 1997-EP637	W	19970212
US 1998-125191	A3	19980813

OTHER SOURCE(S):

MARPAT 127:248093

GI



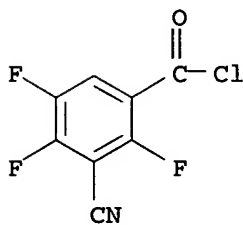
I

AB Title compds. I [R1 = H, alkyl, optionally substituted by OH, OMe, NH2, NHMe, NMe2, or (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; R2 = H, benzyl, alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl, CH=CHCO2R3, CH2CH2CO2R3, CH2CH2CN, CH2CH2COMe, CH2COMe; R3 = Me, Et, R4(NHCHR5CO)n; R4 = H, alkyl, CO2CMe3; R5 = H, alkyl, hydroxyalkyl, aminoalkyl, thioalkyl, carboxyalkyl, benzyl; n = 1, 2; Y = O, S] were prepared for use as antibacterial agents. Thus, I [R1 = OH, R2 = H, Y = O] was prepared by aminating the 7-chloroquinoline. I [R1 = OH, R2 = H, Y = O] had min. inhibitory concns. against a number of bacteria that were superior to those of enrofloxacin.

IT 195532-66-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of diazabicyclononylquinolinecarboxylic acid derivs. as bactericides)

RN 195532-66-2 CAPLUS

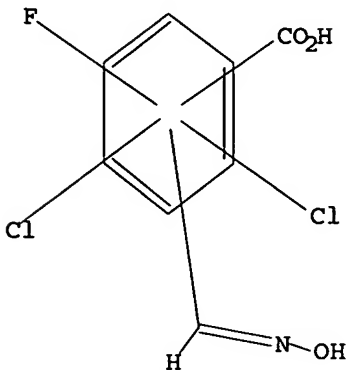
CN Benzoyl chloride, 3-cyano-2,4,5-trifluoro- (9CI) (CA INDEX NAME)





L25 STRUCTURE UPLOADED

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L25 HAS NO ANSWERS  
L25 STR



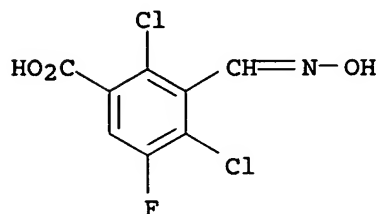
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and chlorination-dehydration of)

RN 214774-57-9 CAPLUS

CN Benzoic acid, 2,4-dichloro-5-fluoro-3-[(hydroxyimino)methyl]- (9CI) (CA  
INDEX NAME)

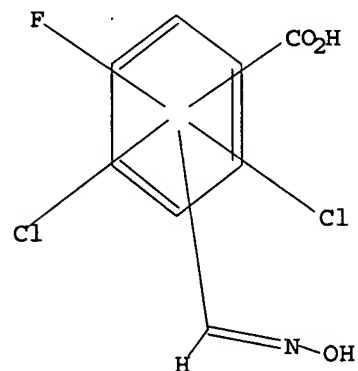


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L25 STRUCTURE UPLOADED

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L25 HAS NO ANSWERS  
L25 STR



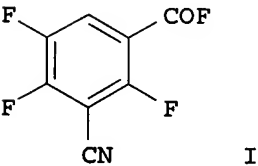
Structure attributes must be viewed using STN Express query preparation.

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ACCESSION NUMBER: 1998:709043 CAPLUS  
DOCUMENT NUMBER: 129:316044  
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and intermediates for its production  
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321
			US 2002-227310	A3 20020826

GI



AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

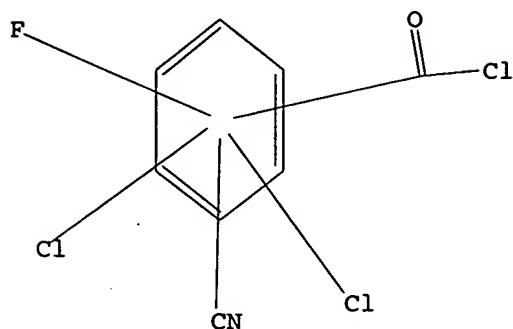
IT 214774-57-9P

L1 . . . STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

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REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 12:42:18 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5 TO 234

PROJECTED ANSWERS: 0 TO 0

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L3 0 L2

=> s l1 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 12:42:27 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

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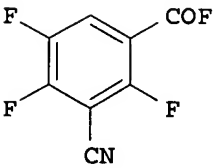
L5 2 L4

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L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1998:709043 CAPLUS  
DOCUMENT NUMBER: 129:316044  
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and  
intermediates for its production  
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
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US 6706918	B2	20040316		
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US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
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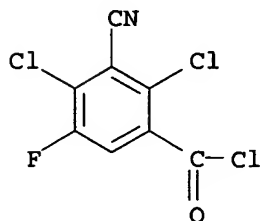
GI



AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic

acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II,  
and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

IT 117528-59-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and fluorination of)  
RN 117528-59-3 CAPLUS  
CN Benzoyl chloride, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:630824 CAPLUS

DOCUMENT NUMBER: 109:230824

TITLE: 8-Cyano-1-cyclopropylquinolonecarboxylic acids as  
antibacterial agents

INVENTOR(S): Schriewer, Michael; Grohe, Klaus; Petersen, Uwe;  
Haller, Ingo; Metzger, Karl Georg; Endermann, Rainer;  
Zeiler, Hans Joachim

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 20 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

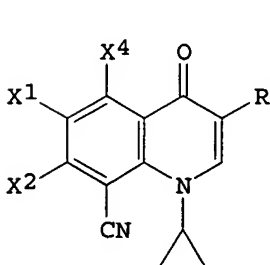
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

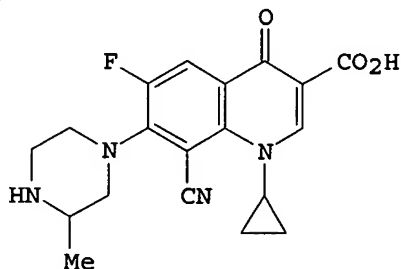
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3702393	A1	19880811	DE 1987-3702393	19870128
US 4908366	A	19900313	US 1988-144884	19880114
EP 276700	A1	19880803	EP 1988-100503	19880115
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
CA 1314544	A1	19930316	CA 1988-557311	19880126
JP 63201170	A2	19880819	JP 1988-14771	19880127
US 5051418	A	19910924	US 1989-434666	19891113
US 5190955	A	19930302	US 1991-645751	19910125
PRIORITY APPLN. INFO.:			DE 1987-3702393	A 19870128
			US 1988-144884	A3 19880114
			US 1989-434666	A3 19891113

OTHER SOURCE(S): CASREACT 109:230824; MARPAT 109:230824

GI



I



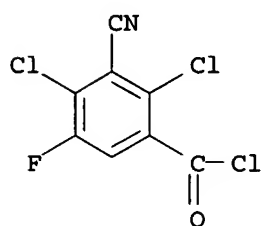
III

AB The title compds. [I; R = CO<sub>2</sub>H, cyano, CO<sub>2</sub>R<sub>1</sub>, CONR<sub>2</sub>R<sub>3</sub>; R<sub>1</sub> = alkyl; R<sub>2</sub> = H, alkyl; R<sub>3</sub> = R<sub>2</sub>, (un)substituted Ph; X<sub>1</sub> = H, NO<sub>2</sub>, alkyl, halo; X<sub>2</sub> = heterocyclyl; X<sub>4</sub> = H, halo, alkyl] were prepared as antibacterial agents (no data). 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOCH<sub>2</sub>CO<sub>2</sub>Et (preparation given) was heated 2 h at 150° with HC(OEt)<sub>3</sub> in Ac<sub>2</sub>O to give 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOC(:CHR<sub>4</sub>)CO<sub>2</sub>Et (II; R<sub>4</sub> = OEt) which was stirred 2 h with cyclopropylamine in EtOH to give II (R = cyclopropylamino). The latter was stirred 24 h in dioxane containing KOCMe<sub>3</sub> to give, after saponification, I (R = CO<sub>2</sub>H, X<sub>1</sub> = F, X<sub>2</sub> = Cl, X<sub>4</sub> = H) which was heated 3 h in dioxane with 2-methylpiperazine to give title compound III. Tablets were prepared each containing III 583.0, cellulose 55.0, starch 72.0, polyvinylpyrrolidone 30.0, silica 5.0, and Mg stearate 5.0 mg coated with poly(O-hydroxypropyl-O-methyl)cellulose 6.0, Macrogol 4000 2.0, TiO<sub>2</sub> 2.0 mg, and polyethyleneglycol (no amount given).

IT 117528-59-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and reaction of, in preparation of antibacterial agents)

RN 117528-59-3 CAPLUS

CN Benzoyl chloride, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



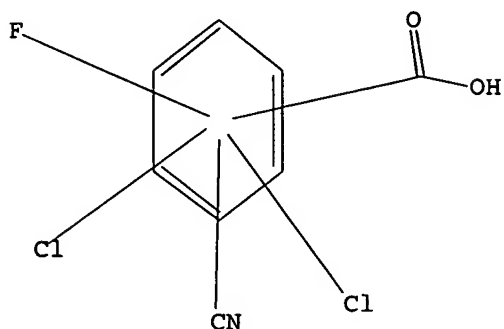
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L9. STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 13:42:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 132 TO 668

PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

L11 0 L10

=> s 19 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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FULL SCREEN SEARCH COMPLETED - 260 TO ITERATE

100.0% PROCESSED 260 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

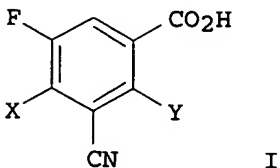
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L13 3 L12  
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L13 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1999:101296 CAPLUS  
DOCUMENT NUMBER: 130:139168  
TITLE: Preparation of 3-cyano-2,4-dihalo-5-fluorobenzoic acid  
by hydrolysis of the corresponding amides, nitriles,  
or esters.  
INVENTOR(S): Hallenbach, Werner; Marhold, Albrecht  
PATENT ASSIGNEE(S): Bayer A.-G., Germany  
SOURCE: Ger. Offen., 18 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19733243	A1	19990204	DE 1997-19733243	19970801
CA 2298805	AA	19990211	CA 1998-2298805	19980718
WO 9906360	A1	19990211	WO 1998-EP4468	19980718
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9891544	A1	19990222	AU 1998-91544	19980718
AU 744367	B2	20020221		
EP 1001929	A1	20000524	EP 1998-943740	19980718
EP 1001929	B1	20030326		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
BR 9811579	A	20000822	BR 1998-11579	19980718
JP 2001512098	T2	20010821	JP 2000-505122	19980718
NZ 502587	A	20020531	NZ 1998-502587	19980718
AT 235461	E	20030415	AT 1998-943740	19980718
PT 1001929	T	20030731	PT 1998-943740	19980718
ES 2190602	T3	20030801	ES 1998-943740	19980718
CN 1125042	B	20031022	CN 1998-807849	19980718
RU 2214998	C2	20031027	RU 2000-105245	19980718
US 6462218	B1	20021008	US 2000-463272	20000124
MX 200000861	A	20001109	MX 2000-861	20000125
HK 1030598	A1	20040702	HK 2001-101537	20010302
PRIORITY APPLN. INFO.:			DE 1997-19733243	A 19970801
			WO 1998-EP4468	W 19980718
OTHER SOURCE(S):			CASREACT 130:139168	
GI				



AB Title compds. (I; X, Y = halo) were prepared by hydrolysis of the  
corresponding 3-cyano-2,4-dihalo-5-fluorobenzamides, 1,3-dicyano-2,4-  
dihalo-5-fluorobenzenes, or 3-cyano-2,4-dihalo-5-fluorobenzoate esters.  
Thus, 3-cyano-2,4-dichloro-5-fluorobenzamide was refluxed 3 h with concentrate  
aqueous HCl to give 3-cyano-2,4-dichloro-5-fluorobenzoic acid.

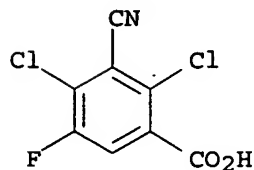
IT 117528-58-2P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
(Preparation)

(preparation of 3-cyano-2,4-dihalo-5-fluorobenzoic acid by hydrolysis of the  
corresponding amides, nitriles, or esters)

RN 117528-58-2 CAPLUS

CN Benzoic acid, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



L13 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:709043 CAPLUS

DOCUMENT NUMBER: 129:316044

TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and  
intermediates for its production

INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

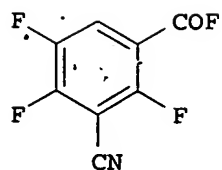
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
DE 19717231	A1	19981029	DE 1997-19717231	19970424
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AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R:	AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE			
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321
			US 2002-227310	A3 20020826

GI



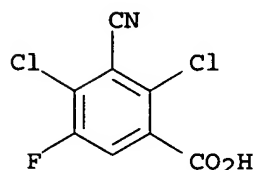
I

AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

IT 117528-58-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 117528-58-2 CAPLUS

CN Benzoic acid, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:630824 CAPLUS

DOCUMENT NUMBER: 109:230824

TITLE: 8-Cyano-1-cyclopropylquinolonecarboxylic acids as antibacterial agents

INVENTOR(S): Schriewer, Michael; Grohe, Klaus; Petersen, Uwe; Haller, Ingo; Metzger, Karl Georg; Endermann, Rainer; Zeiler, Hans Joachim

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 20 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

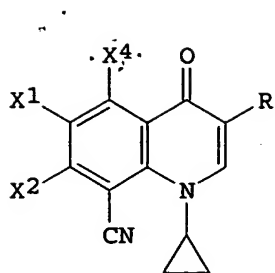
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

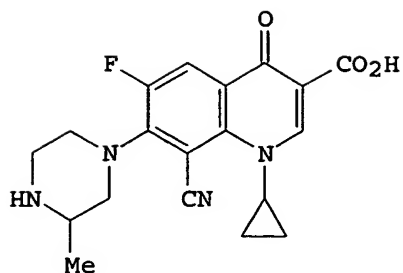
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3702393	A1	19880811	DE 1987-3702393	19870128
US 4908366	A	19900313	US 1988-144884	19880114
EP 276700	A1	19880803	EP 1988-100503	19880115
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
CA 1314544	A1	19930316	CA 1988-557311	19880126
JP 63201170	A2	19880819	JP 1988-14771	19880127
US 5051418	A	19910924	US 1989-434666	19891113
US 5190955	A	19930302	US 1991-645751	19910125
PRIORITY APPLN. INFO.:			DE 1987-3702393	A 19870128
			US 1988-144884	A3 19880114
			US 1989-434666	A3 19891113

OTHER SOURCE(S): CASREACT 109:230824; MARPAT 109:230824

GI



I



III

AB The title compds. [I; R = CO<sub>2</sub>H, cyano, CO<sub>2</sub>R<sub>1</sub>, CONR<sub>2</sub>R<sub>3</sub>; R<sub>1</sub> = alkyl; R<sub>2</sub> = H, alkyl; R<sub>3</sub> = R<sub>2</sub>, (un)substituted Ph; X<sub>1</sub> = H, NO<sub>2</sub>, alkyl, halo; X<sub>2</sub> = heterocyclyl; X<sub>4</sub> = H, halo, alkyl] were prepared as antibacterial agents (no data). 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOCH<sub>2</sub>CO<sub>2</sub>Et (preparation given) was heated 2 h at 150° with HC(OEt)<sub>3</sub> in Ac<sub>2</sub>O to give 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOC(:CHR<sub>4</sub>)CO<sub>2</sub>Et (II; R<sub>4</sub> = OEt) which was stirred 2 h with cyclopropylamine in EtOH to give II (R = cyclopropylamino). The latter was stirred 24 h in dioxane containing KO<sup>t</sup>Me<sub>3</sub> to give, after saponification, I (R = CO<sub>2</sub>H, X<sub>1</sub> = F, X<sub>2</sub> = Cl, X<sub>4</sub> = H) which was heated 3 h in dioxane with 2-methylpiperazine to give title compound III. Tablets were prepared each containing III 583.0, cellulose 55.0, starch 72.0, polyvinylpyrrolidone 30.0, silica 5.0, and Mg stearate 5.0 mg coated with poly(O-hydroxypropyl-O-methyl)cellulose 6.0, Macrogol 4000 2.0, TiO<sub>2</sub> 2.0 mg, and polyethyleneglycol (no amount given).

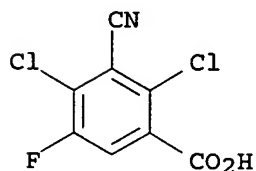
IT 117528-58-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antibacterial agents)

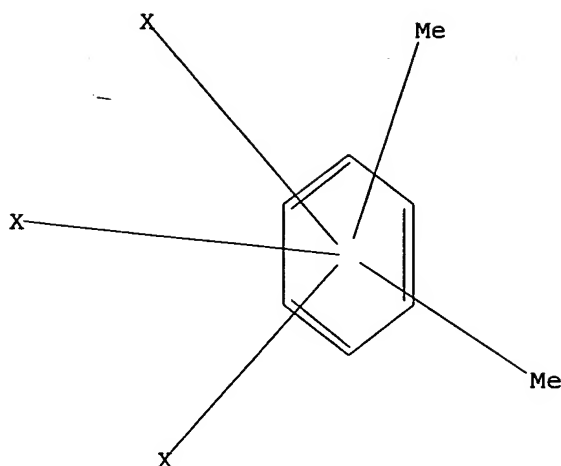
RN 117528-58-2 CAPLUS

CN Benzoic acid, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



L8

STR



Structure attributes must be viewed using STN Express query preparation.

=> s l8 sss full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 16:21:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1832446 TO ITERATE

42.4% PROCESSED 776666 ITERATIONS

101 ANSWERS

54.6% PROCESSED 1000000 ITERATIONS

109 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.31

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 1832446 TO 1832446

PROJECTED ANSWERS: 157 TO 241

L9 109 SEA SSS FUL L8

L10 37 L9

=> s l10 and py<1997

17513355 PY<1997

L11 28 L10 AND PY<1997

=> d 1-28 ibib abs hitstr

L11 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1962:416724 CAPLUS

DOCUMENT NUMBER: 57:16724

ORIGINAL REFERENCE NO.: 57:3345h-i,3346a-b

TITLE: Molecular compounds analogous to phenoquinone type

AUTHOR(S): Kumamoto, Sanetada

CORPORATE SOURCE: Univ. Kagoshima

SOURCE: Kogyo Kagaku Zasshi (1961), 64, 1812-16

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

AB Eight chlorinated and methylated p-quinones and twelve phenols, mainly chlorinated, were prepared. These p-quinones (1 mole) and phenols (2 moles) were dissolved in benzene, CCl<sub>4</sub>, CHCl<sub>3</sub>, CS<sub>2</sub>, and left for several days. Several kinds of mol. compds. (I) were formed as crystals with beautiful colors, by evaporating the solvent. Among p-quinones, tetramethyl-p-benzoquinone was easiest to form I. However, the formation of I became more difficult as H atoms of the nucleus of p-benzoquinone were substituted with Cl atoms. Some of I were observed to change suddenly from their own proper color to yellow at their resp. discoloration temperature even below the m.p. This discoloration temperature is postulated as the temperature where the intermol. H bond is cut off with decomposition to individual constituents. The existence of intermol. H bond in the crystalline state was recognized by the infrared spectra. These crystals were mol. compds. analogous to phenoquinones formed by intermol. H bonds between p-quinones (1 mole) and phenols (2 moles).

IT 856302-22-2, p-Benzoquinone, tetramethyl-, compound with 2,4,6-trichloro-3,5-xyleneol 856303-09-8, p-Benzoquinone, 2,5-dichloro-3,6-dimethoxy-, compound with 2,4,6-trichloro-3,5-xyleneol 859803-13-7, 3,5-Xyleneol, 2,4,6-trichloro-, compound with trichlormethyl-p-benzoquinone 859803-19-3, 3,5-Xyleneol, 2,4,6-trichloro-, compound with methyl-p-benzoquinone 859803-22-8, 3,5-Xyleneol, 2,4,6-trichloro-, compound with 2,5-dimethyl-p-benzoquinone 859803-26-2, 3,5-Xyleneol, 2,4,6-trichloro-, compound with 2,5-dichloro-3,6-dimethyl-p-benzoquinone (preparation of)

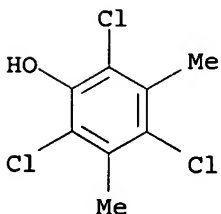
RN 856302-22-2 CAPLUS

CN p-Benzoquinone, tetramethyl-, compd. with 2,4,6-trichloro-3,5-xyleneol (7CI) (CA INDEX NAME)

CM 1

CRN 6972-47-0

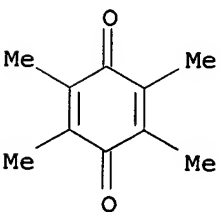
CMF C8 H7 Cl3 O



CM 2

CRN 527-17-3

CMF Cl0 H12 O2



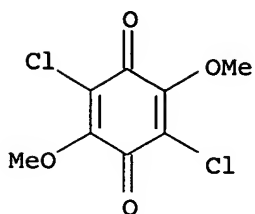
RN 856303-09-8 CAPLUS

CN p-Benzoquinone, 2,5-dichloro-3,6-dimethoxy-, compd. with 2,4,6-trichloro-3,5-xyleneol (7CI) (CA INDEX NAME)

CM 1

CRN 7210-71-1

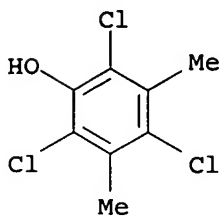
CMF C8 H6 Cl2 O4



CM 2

CRN 6972-47-0

CMF C8 H7 Cl3 O



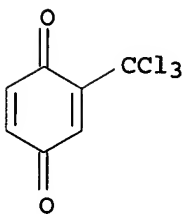
RN 859803-13-7 CAPLUS

CN 3,5-Xylenol, 2,4,6-trichloro-, compd. with trichlormethyl-p-benzoquinone  
(7CI) (CA INDEX NAME)

CM 1

CRN 856302-00-6

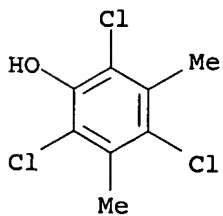
CMF C7 H3 Cl3 O2



CM 2

CRN 6972-47-0

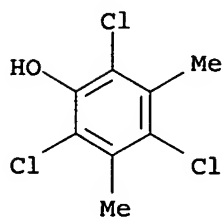
CMF C8 H7 Cl3 O



RN 859803-19-3 CAPLUS  
CN 3,5-Xylenol, 2,4,6-trichloro-, compd. with methyl-p-benzoquinone (7CI)  
(CA INDEX NAME)

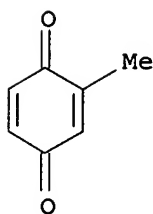
CM 1

CRN 6972-47-0  
CMF C8 H7 Cl3 O



CM 2

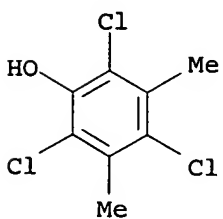
CRN 553-97-9  
CMF C7 H6 O2



RN 859803-22-8 CAPLUS  
CN 3,5-Xylenol, 2,4,6-trichloro-, compd. with 2,5-dimethyl-p-benzoquinone  
(7CI) (CA INDEX NAME)

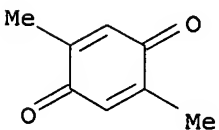
CM 1

CRN 6972-47-0  
CMF C8 H7 Cl3 O



CM 2

CRN 137-18-8  
CMF C8 H8 O2

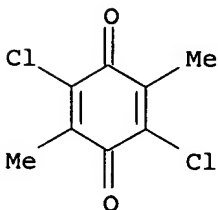




RN 859803-26-2 CAPLUS  
CN 3,5-Xylenol, 2,4,6-trichloro-, compd. with 2,5-dichloro-3,6-dimethyl-p-benzoquinone (7CI) (CA INDEX NAME)

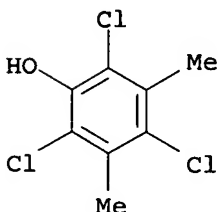
CM 1

CRN 46010-98-4  
CMF C8 H6 Cl2 O2



CM 2

CRN 6972-47-0  
CMF C8 H7 Cl3 O



L11 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:69181 CAPLUS  
DOCUMENT NUMBER: 50:69181  
ORIGINAL REFERENCE NO.: 50:12856c-g  
TITLE: The action of aluminum chloride on alkylbenzenes  
AUTHOR(S): Nightingale, Dorothy V.; Shackelford, James M.  
CORPORATE SOURCE: Univ. of Missouri, Columbia  
SOURCE: Journal of the American Chemical Society (1956  
) , 78, 1225-7  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

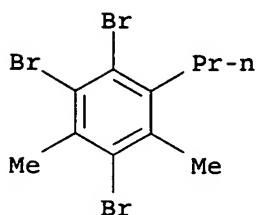
AB cf. C.A. 49, 14656e. 2,4-Me2C6H3COEt subjected to a Wolff-Kischner reduction yielded 68% 2,4-Me2C6H3Pr (I), b16 90-1°, nD25 1.4980; 2,4-Me2C6(NO2)3Pr (Ia), m. 108.5-109°; 2,4-Me2C6Br3Pr, oil. 2,4-Me2C6H3C(OH)Me2 reduced with hydrogen and Cu-Cr2O3 catalyst gave 2,4-Me2C6H3CHMe2 (II), b17 87-8°, nD20 1.4998; 2,4-Me2C6(NO2)3CHMe2 (III), m. 99-9.5°; 2,4-Me2C6Br3CHMe2, m. 63-4°. m-Xylene (IV) and iso-PrCl gave in the usual manner 1,3-Me2C6H3CHMe2 (V), b18 86-7°, nD25 1.4955, containing 13% 1,3,4-trialkylbenzene; 1,3-Me2C6(NO2)3CHMe2 (VI), m. 115.5-16°. IV (65 g.) and 31 g. AlCl3 treated slowly with stirring with 39 g. PrCl below 20°, and the mixture kept at room temperature overnight and decomposed with ice and HCl yielded 11 g. V, b. 80-6° (VI, m. 115-16°), 4 g. distillate, b. 86-8°, and 18 g. I, b. 88-91° (Ia, m. 98.5-99°). IV (200 cc.), 48 g. iso-PrOH, and 400 cc. 85% H2SO4 yielded 37 g. hydrocarbon, b15 85-6°, nD24 1.5004; the trinitro derivative, m. 177-8°, did not depress the m.p. of 1,3-Me2C6H(NO2)3. I (135 g.) treated with stirring on the steam bath with 29 g. AlCl3, the complex decomposed with iced HCl, and the hydrocarbon distilled yielded 22 g. IV, b16 75°, 5 g. mixed distillate, b16 85-9°, 35 g., b16

89-90°, nD<sub>22</sub> 1.4965 (III, m. 99-9.5°), 12 g. distillate, b<sub>16</sub> 90-1°, 12 g. distillate, b<sub>16</sub> 91-110°, and 20 g. distillate, b<sub>16</sub> 110-20°. II (55 g.) and 12 g. AlCl<sub>3</sub> gave similarly 19 g. V containing 13% II. 1,2,4-C<sub>6</sub>H<sub>3</sub>Pr<sub>3</sub> (VI) brominated yielded an oil, while p-C<sub>6</sub>H<sub>4</sub>Pr<sub>2</sub> gave p-C<sub>6</sub>Br<sub>4</sub>Pr<sub>2</sub>, m. 107-8°. VI (29 g.) treated with 10 g. AlCl<sub>3</sub> and the hydrocarbon fractionated gave a fraction, b. 130-40°, which contained mainly the 1,3,5-isomer of VI; 1,3,5-Pr<sub>3</sub>C<sub>6</sub>Br<sub>3</sub>, m. 112-13°; 1,3,5-Pr<sub>3</sub>C<sub>6</sub>(NO<sub>2</sub>)<sub>3</sub>, m. 123-4°.

IT 859785-24-3, m-Xylene, 2,4,5-tribromo-6-propyl-  
859785-26-5, m-Xylene, 2,4,6-tribromo-5-propyl-  
(preparation of)

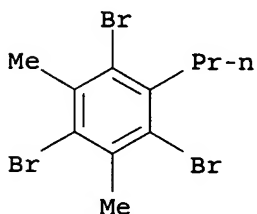
RN 859785-24-3 CAPLUS

CN m-Xylene, 2,4,5-tribromo-6-propyl- (5CI) (CA INDEX NAME)



RN 859785-26-5 CAPLUS

CN m-Xylene, 2,4,6-tribromo-5-propyl- (5CI) (CA INDEX NAME)



L11 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:27703 CAPLUS

DOCUMENT NUMBER: 50:27703

ORIGINAL REFERENCE NO.: 50:5542d-i,5543a-i,5544a-e

TITLE: Additive compounds as possible intermediates in substitution processes. II

AUTHOR(S): Bell, F.

CORPORATE SOURCE: Heriot-Watt Coll., Edinburgh, UK

SOURCE: Journal of the Chemical Society (1955)  
2376-83

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

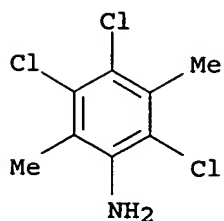
AB cf. C.A. 50, 898i. Chlorination of many sulfonanilides readily gave cyclohexene derivs. The reactions of these compds. were discussed. The halogenation of 3,4-xylylene (I) was studied. N-p-Toluenesulfonyl-p-toluidine (II) with Cl in either AcOH or CHCl<sub>3</sub>, or with SO<sub>2</sub>Cl<sub>2</sub> alone or in CHCl<sub>3</sub> gave 3,3,5,6-tetrachloro-1-methyl-4-p-toluenesulfonyliminocyclohexene (III). Thus 10 g. II added slowly to excess SO<sub>2</sub>Cl<sub>2</sub>, the excess SO<sub>2</sub>Cl<sub>2</sub> removed in vacuo, the residual oil dissolved in AcOH, and precipitated by addition of H<sub>2</sub>O gave 4.7 g. III, m. 184° (from AcOH, or C<sub>6</sub>H<sub>6</sub>). III reacted with piperidine but gave no definite compound. Excess Zn dust added to a refluxing AcOH solution of III gave 2-chloro-N-(p-toluenesulfonyl)-toluidine (IIIa). III heated at 200° until gas evolution ceased gave 2,3,6-trichloro-N-(p-toluenesulfonyl)-p-toluidide (IV), m. 160° (from AcOH). IV in cold H<sub>2</sub>SO<sub>4</sub> gave 2,3,6-trichloro-p-toluidine (V) almost quantitatively, m. 60-2°; Ac derivative, m. 196°; di-Ac derivative, m. 150°. III reacted vigorously with C<sub>5</sub>H<sub>5</sub>N and on acidification gave a poor yield of IV. III (2 g.) heated 1.5 hrs. at 150° with 4

cc. H<sub>2</sub>SO<sub>4</sub> and 4 cc. H<sub>2</sub>O gave a black tar, and addition of excess of aqueous NH<sub>3</sub> yielded V. Addition of PhNH<sub>2</sub> to III gave an impure solid, m. 135°. III dissolved during 3 hrs. in refluxing EtOH gave 1,1,3,4-tetrachloro-6(?)-ethoxy-5-methyl-2-p-toluenesulfonyliminocyclohexane, m. 195°, and IV. A similar reaction with MeOH gave the MeO analog (VI), m. 187° (from EtOH). Reduction of VI by Zn dust and AcOH gave 2-chloro-N-(p-toluenesulfonyl)-p-toluidine, m. 220° (decomposition), and some IV. Solution in warm C<sub>5</sub>H<sub>5</sub>N gave almost quant. conversion to 2,6-dichloro-3-methoxy-N-(p-toluenesulfonyl)-p-toluidine (VII) m. 190° (from AcOH). VII was also obtained by use of PhNH<sub>2</sub> but was accompanied by sticky, red decomposition products. Aceto-p-toluidide (VIII) chlorinated by Cohen and Dakin's method [J. Chemical Society 81, 1337(1902)] gave a crude product, m. about 179°, which on hydrolysis in EtOH-HCl gave a base, m. 35-47°. This was purified and reacylated to yield the Ac and di-Ac derivs. of V. With p-tosyl chloride it gave IV. Similarly 2,3,6-trichloro-N-benzenesulfonyl-p-toluidine (IX) was obtained, m. 169° (from EtOH). In a typical experiment 5 g. VIII gave 1.9 g. of the 2,6-dinitro derivative, m. 190°. Various proportions of HNO<sub>3</sub> and HCl were used but in no case was any of the trichloro derivative isolated. 2,6-Dichloro-p-toluidine gave the N-benzenesulfonyl derivative, m. 169° (from AcOH), and the N-(p-toluenesulfonyl) derivative, m. 180° (from C<sub>6</sub>H<sub>6</sub>). IIIa in C<sub>5</sub>H<sub>5</sub>N on treatment with N-bromosuccinimide gave 2-bromo-6-chloro-N-(p-toluenesulfonyl)-p-toluidine, m. 180°. It was unchanged after treatment with Zn dust in refluxing AcOH. II in CHCl<sub>3</sub> treated with 1 mole Br gave the 2-bromo derivative (X), m. 118° (from EtOH). II in C<sub>5</sub>H<sub>5</sub>N with 2 moles N-bromosuccinimide yielded 2,6-dibromo-N-(p-toluenesulfonyl)-p-toluidine (XI), m. 179-80° (from AcOH). X and XI did not react with Zn dust in AcOH. p-Toluidine treated with Cl in AcOH gave thick, dark oils. N-Benzenesulfonyl-p-toluidine (XII) in CHCl<sub>3</sub> treated with excess Cl yielded 4-benzenesulfonylimino-3,3,5,6-tetrachloro-1-methylcyclohexene (XIII), m. 164°. XIII reacted vigorously with C<sub>5</sub>H<sub>5</sub>N to give IX in small yield. XIII with PhNH<sub>2</sub> gave a mixture from which was obtained a powder, m. 158° (decomposition) (from AcOH), which appeared to have been produced by loss of HCl from XIII. The o-isomer (XIV) of XII (4 g.) was similarly chlorinated to give 6-benzenesulfonylimino-3,3,4,5-tetrachloro-1-methylcyclohexene (XV), m. 166° (from AcOH). The yield of XV was not improved by using N-benzenesulfonyl-4-chloro-o-toluidine (XVI) as starting material. XV treated with Zn in AcOH yielded XVI. XV with PhNH<sub>2</sub> gave 4-anilino-N-benzenesulfonyl-5,6-dichloro-o-toluidine, m. 207° (from AcOH), and was hydrolyzed by cold H<sub>2</sub>SO<sub>4</sub> to 4-anilino-5,6-dichloro-o-toluidine, m. 115° (from EtOH). XV heated above the m.p. gave N-benzenesulfonyl-4,5,6-trichloro-o-toluidine, m. 159°. N-p-Toluene sulfonyl-o-toluidine (XVII) (14 g.) submitted to the same process gave 4 g. 4-chloro derivative (XVIII) and an oil. N-Acetyl-2-chloro-p-toluidine gave 1 g. 2,6-dichloro amide and an uncrystallizable oil. When excess SO<sub>2</sub>Cl<sub>2</sub> was added to the sulfonamide, and after the initial reaction, excess SO<sub>2</sub>Cl<sub>2</sub> removed and the residue dissolved in EtOH or AcOH, the following results were obtained: XVII (5 g.) gave 4 g. XVIII, m. 144°; XIV (4 g.) gave 2.6 g. 4-chloro derivative and a small yield of XV; N-benzenesulfonyl-m-toluidine gave an almost quant. yield of the dichloro derivative, m. 116°; N-p-toluenesulfonyl-m-toluidine gave crude 2,4-dichloro-N-p-toluenesulfonyl-m-toluidine (XIX), pure XIX, prepared from 2,4-dichloro-p-toluidine, m. 145° (from AcOH); XII (5 g.) gave 2.5 g. 2-Cl derivative and an oil; N-p-toluenesulfonyl-p-anisidine gave the dichloro derivative (XX), m. 166°, XX was hydrolyzed to the dichloro base, m. 75°. 2,3-Xylidine with p-tosyl chloride in C<sub>5</sub>H<sub>5</sub>N yielded N-p-toluenesulfonyl-2,3-xylidine (XXI), m. 147° (from EtOH). XXI in CHCl<sub>3</sub> treated with Cl gas gave an almost quant. yield of 4-chloro-N-p-toluenesulfonyl-2,3-xylidine (XXII), m. 142° (from EtOH). XXII, alternatively prepared from 4-chloro-2,3-xylidine and p-tosyl chloride in C<sub>5</sub>H<sub>5</sub>N, was unchanged after 2 days in concentrated H<sub>2</sub>SO<sub>4</sub>. XXI with excess SO<sub>2</sub>Cl<sub>2</sub> gave 4,6-dichloro-N-p-toluenesulfonyl-2,3-xylidine, m. 174°, and a main crop of 3,3,4,5-tetrachloro-1,2-dimethyl-6-p-toluenesulfonyliminocyclohexene (XXIII), m. 128-30°. XXIII refluxed 3 hrs. in EtOH, by solution in C<sub>5</sub>H<sub>5</sub>N, or at 190° gave 4,5,6-trichloro-N-p-toluenesulfonyl-2,3-xylidine, m. 206° (from AcOH). Reduction of XXIII in AcOH with Zn dust gave XXII, and with PhNH<sub>2</sub>

it reacted to give 4-anilino-5,6-dichloro-N-p-toluenesulfonyl-2,3-xylidine, m. 205° (from AcOH) Cl passed into N-p-toluenesulfonyl-3,4-xylidine (XXIV) in CHCl<sub>3</sub> gave a small crop of unchanged XXIV and an oil. When XXIV (5 g.) was treated with SO<sub>2</sub>Cl<sub>2</sub> it yielded 0.6 g. putative 3,3,5,5,6-pentachloro-4-p-toluenesulfonylimino-1,2-dimethylcyclohexene (XXV), m. 187° (decomposition) (from AcOH). XXV yielded an uncrystallizable material on thermal decomposition, and on reduction with Zn in AcOH a complex mixture N-Acetyl-3,4-xylidine (XXVI) on chlorination yielded a monochloro derivative, m. 153°. Passage of excess Cl into a CHCl<sub>3</sub> solution of XXVI led to oils. 2,4-Xylidine with p-tosyl chloride gave N-p-toluenesulfonyl-2,4-xylidine (XXVII), m. 109° (from EtOH). XXVII with excess SO<sub>2</sub>Cl<sub>2</sub> gave a low yield of a trichloro derivative (XXVIII), m. 163° (decomposition) (from AcOH). Cl passed into a CHCl<sub>3</sub> solution of XXVII gave a small amount of XXVIII and a small crop of 3,5,6-trichloro-N-p-toluenesulfonyl-2,4-xylidine, m. 152° (from AcOH). Commercial NaOCl solution added to XXVII in AcOH at 50° yielded 6-chloro-N-p-toluenesulfonyl-2,4-xylidine, m. 158°. N-Benzenesulfonyl-2,4-xylidine (XXIX) (8 g.) with SO<sub>2</sub>Cl<sub>2</sub> yielded a somewhat impure trichloro derivative with highest m.p. at 198-202°. Chlorination of XXIX in CHCl<sub>3</sub> gave similar results. p-Toluenesulfonyl-2,5-xylidine (XXX) similarly treated with SO<sub>2</sub>Cl<sub>2</sub> and the oil remaining after removal of the solvent taken up in AcOH gave crop A and the filtrate treated with H<sub>2</sub>O gave a gummy product. This gum upon repeated crystallization from EtOH gave a tetrachloro derivative (XXXI), m. 152°. Reduction of XXXI by Zn dust and AcOH gave 4-chloro-N-p-toluenesulfonyl-2,5-xylidine (XXXII), m. 145° (from EtOH). XXXI vigorously reacted with C<sub>5</sub>H<sub>5</sub>N but gave no recognizable product as did treatment with cold concentrated H<sub>2</sub>SO<sub>4</sub>. Crop A yielded putative 3,3,5-trichloro-6-p-toluenesulfonamido-1,4-dimethylcyclohexa-1,4-diene (XXXIII), m. 132°. Solution of XXXIII in hot EtOH gave 3,4,6-trichloro-N-p-toluenesulfonyl-2,5-xylidine (XXXIV), m. 167°, also obtained in small yield from the products of thermal decomposition of, and on suspension of XXXIII in cold concentrated H<sub>2</sub>SO<sub>4</sub>. Upon addition of XXXIII to C<sub>5</sub>H<sub>5</sub>N, the solution became momentarily bright yellow and then faded; addition of dilute HCl gave 4,6-dichloro-N-p-toluenesulfonyl-2,5-xylidine (XXXV), m. 125-6° (from EtOH). XXXV gave the dichloro base on hydrolysis, m. 166-8°, and this without further purification was acetylated to N-acetyl-4,6-dichloro-2,5-xylidine (XXXVI), m. 166-8° (from EtOH), alternatively prepared from N-acetyl-2,5-xylidine and SO<sub>2</sub>Cl<sub>2</sub>. Reduction of XXXIII in refluxing AcOH with Zn dust produced a material, m. 117-20°, apparently a mixture of mono- and trichloro derivs., for after dissolution in H<sub>2</sub>SO<sub>4</sub> there was obtained XXXII. XXXIV was not reduced with Zn dust in refluxing AcOH, but on dissolution in H<sub>2</sub>SO<sub>4</sub> readily gave the amine, m. 206°. Addition of SO<sub>2</sub>Cl<sub>2</sub> to XXX gave an almost theoretical yield of XXXII. Cl passed into a solution of 5 g. XXX in CHCl<sub>3</sub> gave 1.2 g. crude XXXII and 1 g. XXXIII. XXX (2 g.) treated with excess NaOCl in AcOH at 50° yielded XXXII contaminated with unchanged material. Cl passed into a solution of N-p-toluenesulfonyl-2,6-xylidine (XXXVII) in CHCl<sub>3</sub> gave the monochloro derivative (XXXVIII), m. 158° (from AcOH or EtOH). XXXVII (4 g.) with excess SO<sub>2</sub>Cl<sub>2</sub> gave 1.9 g. XXXVIII. XXVI in AcOH treated with Br gave after 24 hrs. a product which was essentially N-acetyl-6-bromo-3,4-xylidine (XXXIX), m. 164° (from EtOH). Hydrolysis of XXXIX with refluxing EtOH-HCl gave 6-bromo-3,4-xylidine; p-toluenesulfonyl derivative (XL), m. 122° (from EtOH). Addition of Br in CHCl<sub>3</sub> to a CHCl<sub>3</sub> solution of XXIV gave XL in almost quant. yield. Heating XXIV in CHCl<sub>3</sub> with Br gave XL together with the HBr salt of 2,6-dibromo-3,4-xylidine. Addition of Br to XXIV in cold C<sub>5</sub>H<sub>5</sub>N gave the 2,6-dibromo derivative (XLI), m. 165° (from EtOH). Dissolution of XLI in cold H<sub>2</sub>SO<sub>4</sub> gave the 2,6-dibromo amine; Ac derivative (XLII), m. 198°. XLII crystallized from EtOH as needles, which in contact with solvent were slowly transformed into prisms. Passage of Cl into either XXXIX or XL in CHCl<sub>3</sub> led to no crystalline product other than the initial compds. XL was unchanged after treatment with iodine in C<sub>5</sub>H<sub>5</sub>N.

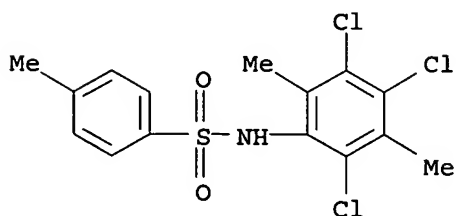
IT 857974-28-8, 2,5-Xylidine, 3,4,6-trichloro- 859493-05-3,  
p-Toluenesulfonyl-2',5'-xylidide, 3',4',6'-trichloro- 859493-26-8  
, p-Toluenesulfonyl-2',3'-xylidide, 4',5',6'-trichloro- 859791-74-5  
, p-Toluenesulfonyl-2',4'-xylidide, 3',5',6'-trichloro-  
(preparation of)  
RN 857974-28-8 CAPLUS

CN 2,5-Xylidine, 3,4,6-trichloro- (5CI) (CA INDEX NAME)



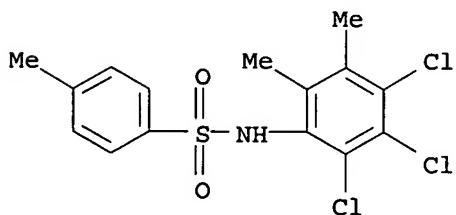
RN 859493-05-3 CAPLUS

CN p-Toluenesulfono-2',5'-xylidide, 3',4',6'-trichloro- (5CI) (CA INDEX NAME)



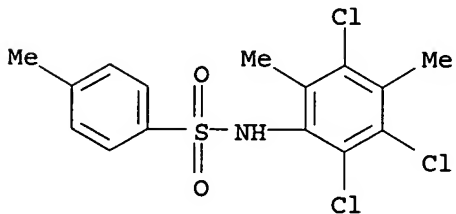
RN 859493-26-8 CAPLUS

CN p-Toluenesulfono-2',3'-xylidide, 4',5',6'-trichloro- (5CI) (CA INDEX NAME)



RN 859791-74-5 CAPLUS

CN p-Toluenesulfono-2',4'-xylidide, 3',5',6'-trichloro- (5CI) (CA INDEX NAME)



L11 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1955:77678 CAPLUS

DOCUMENT NUMBER: 49:77678

ORIGINAL REFERENCE NO.: 49:14656e-i,14657a-b

TITLE: The action of aluminum chloride on alkylbenzenes. IV

AUTHOR(S): Nightingale, Dorothy V.; Shackelford, James M.

CORPORATE SOURCE: Univ. of Missouri, Columbia

SOURCE: Journal of the American Chemical Society (1954), 76, 5767-70

CODEN: JACSAT; ISSN: 0002-7863

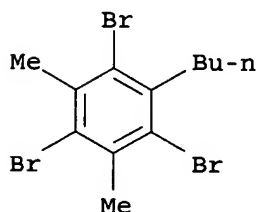
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB cf. C.A. 49, 228a. When 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Bu (I), 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>EtMe (II), and 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CHMe<sub>2</sub> (III) are warmed with AlCl<sub>3</sub>, the C<sub>4</sub>H<sub>9</sub> group migrates to the 5-position without isomerization. The alkylation of m-xylene (IV) with BuCl yielded a mixture of 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Bu (V) and 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>EtMe (VI). The alkylation of IV with EtMeCHCl yielded VI. BuCl (72 g.) added slowly with stirring to 127 g. IV and 60 g. AlCl<sub>3</sub> below 35°, the mixture kept at room temperature overnight, decomposed with iced HCl, extracted with Et<sub>2</sub>O, and the extract washed, dried, and distilled yielded 20 g. VI, b<sub>15</sub> 96-7°, n<sub>25D</sub> 1.4958 (trinitro derivative, m. 90-1°), and 35 g. V, b<sub>15</sub>, 103-4°, n<sub>25D</sub> 1.4947 (trinitro derivative, m. 93-4°). IV (180 g.) alkylated in the same way with 110 g. EtMeCHCl and 95 g. AlCl<sub>3</sub> yielded 125 g. VI, b<sub>15</sub> 95-7°, n<sub>25D</sub> 1.4929 (trinitro derivative, m. 90-1°). IV (250 cc.) and 61 cc. EtMeCHOH treated slowly with stirring with 330 cc. concentrated H<sub>2</sub>SO<sub>4</sub> and 70 cc. H<sub>2</sub>O, the mixture stirred 7 h. at room temperature, and the hydrocarbon layer washed, dried, and distilled gave 68 g. trialkylbenzene, b<sub>28</sub> 106-8°, n<sub>24D</sub> 1.4967, which on nitration yielded only the trinitro derivative of IV, m. 181-2°. The trialkylbenzene (35 g.) warmed 3.5 h. with 8.5 g. AlCl<sub>3</sub> and distilled gave 5 g. distillate b<sub>17</sub> 88-94°, and 12 g. b<sub>17</sub> 94-7°; the nitration product from the 2nd fraction, recrystd. repeatedly, yielded a small amount of the trinitro derivative of VI. PrMgBr from 98 g. PrBr in 200 cc. Et<sub>2</sub>O distilled to remove 100 cc. Et<sub>2</sub>O, the residual solution diluted with 100 cc. C<sub>6</sub>H<sub>6</sub>, treated as rapidly as possible with 160 g. CdCl<sub>2</sub>, refluxed 1 h., the mixture treated with 72 g. 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COCl (VII), refluxed 1 h., decomposed in the usual manner, extracted with Et<sub>2</sub>O, and the C<sub>6</sub>H<sub>6</sub>-Et<sub>2</sub>O solution washed with aqueous Na<sub>2</sub>CO<sub>3</sub> and H<sub>2</sub>O, dried, and distilled yielded 31 g. 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COPr (VIII), b<sub>16</sub> 139°, n<sub>25D</sub> 1.5169; semicarbazone, m. 157°. VIII reduced with H and CuO-Cr<sub>2</sub>O<sub>3</sub> catalyst gave V, b<sub>15</sub> 102-4°, n<sub>25D</sub> 1.4937 (trinitro derivative, m. 95°). VII and Et<sub>2</sub>Cd yielded similarly 48% 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COEt (IX), b<sub>15</sub> 110°, n<sub>25D</sub> 1.5143; semicarbazone, m. 167°. IX (45 g.) and MeMgI yielded in the usual manner 24 g. 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>C(OH)EtMe, b<sub>15</sub> 109-11°, n<sub>24D</sub> 1.5148, which, hydrogenated over CuO-Cr<sub>2</sub>O<sub>3</sub>, yielded 21 g. VI, b<sub>16</sub>, 95-6°, n<sub>24D</sub> 1.4929; trinitro derivative, granules from EtOH, m. 91°. AlCl<sub>3</sub> (23 g.) added to 102 g. I, the mixture warmed on the steam bath 3.5 h., decomposed with iced HCl, and the product isolated in the usual manner yielded 31 g. V, b<sub>16</sub> 103-5° (trinitro derivative, m. 94°; tri-Br derivative, m. 53°). II (133 g.) and 29 g. AlCl<sub>3</sub> gave similarly VI in 2 fractions, b<sub>16</sub> 91-5° (18 g.), and b<sub>16</sub> 95-6° (63 g.); trinitro derivative, granules, m. 91°. III (100 g.) and 20 g. AlCl<sub>3</sub> gave in the same way 20 g. product, b<sub>17</sub> 98-101°, which yielded a trinitro derivative m. 85-6° (either the derivative of 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CHMe<sub>2</sub> or a eutectic mixture). The trinitro derivs. of the hydrocarbons were prepared by adding 2 cc. hydrocarbon slowly with shaking to 10 cc. ice-cold concentrated H<sub>2</sub>SO<sub>4</sub> and 5 cc. fuming HNO<sub>3</sub>, warming the mixture on the water bath at 60-80°, pouring onto ice, and washing and recrystg. the precipitate from EtOH; in this manner were prepared the trinitro derivs. of III, m. 115-16°, and of 3,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CMe<sub>3</sub>, m. 86° with softening at 80-5°. The brominations were carried out with liquid Br in the presence of Fe powder.

IT 859781-62-7, m-Xylene, 2,4,6-tribromo-5-butyl-  
(preparation of)

RN 859781-62-7 CAPLUS

CN m-Xylene, 2,4,6-tribromo-5-butyl- (5CI) (CA INDEX NAME)



ACCESSION NUMBER: 1955:35841 CAPLUS  
DOCUMENT NUMBER: 49:35841  
ORIGINAL REFERENCE NO.: 49:6871f-h  
TITLE: 2,6-Dichloro-3,5-xyleneol  
AUTHOR(S): Gump, Wm. S.; Nikawitz, Edward J.  
CORPORATE SOURCE: Givaudan Corp., Delawanna, NJ  
SOURCE: Journal of the American Chemical Society (1953  
) , 75, 6311-12  
CODEN: JACSAT; ISSN: 0002-7863

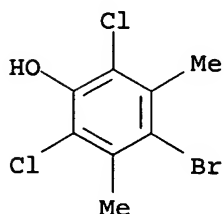
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
OTHER SOURCE(S): CASREACT 49:35841

AB Direct chlorination of 3,5-xyleneol or 2-chloro-3,5-xyleneol yields mixts. containing mostly the 2,4-dichloro derivative (I); benzoate, m. 114-15°. 4-Bromo-3,5-xyleneol (78 g.) in 1.5 l. CCl<sub>4</sub> treated during 10 hrs. with 150 g. Cl at 70-5°, the solution poured into water, the organic layer evaporated, the residue (120 g.) extracted by refluxing 1 hr. with 600 cc. water containing 100 g. NaOH, followed by 3-30 min. extns. with 20 g. NaOH in 500 cc. water, and the combined ests. filtered and acidified with HCl yielded 46.1 g. 4-bromo-2,6-dichloro-3,5-xyleneol (II), m. 183-4°. II (34 g.) and 600 cc. 20% KOH heated to 90°, the solution treated during 2 hrs. with 80 g. Zn dust, heated 3 hrs. at 90°, filtered, the cold filtrate acidified with HCl (ice cooling), filtered, the product refluxed with 100 cc. EtOH containing C, the filtrate diluted with water, and the precipitate (26 g.) distilled yielded 18.3 g. 2,6-dichloro-3,5-xyleneol (III), b<sub>1</sub> 105-10°, m. 87-8°; benzoate, m. 143-5°. I and III have an unpleasant odor. III is much less active bactericidally than I.

IT 408314-44-3, 3,5-Xyleneol, 4-bromo-2,6-dichloro-  
(preparation of)

RN 408314-44-3 CAPLUS

CN Phenol, 4-bromo-2,6-dichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1954:10924 CAPLUS  
DOCUMENT NUMBER: 48:10924  
ORIGINAL REFERENCE NO.: 48:1989d-g  
TITLE: Chloramines as a source of iodine chloride.  
Preparation of iodophenols, -naphthols and -aromatic  
ethers by means of a chloramine and an iodide  
AUTHOR(S): Jones, Brynmor; Richardson, Eileen N.  
CORPORATE SOURCE: Univ. Coll., Hull, UK  
SOURCE: Journal of the Chemical Society (1953)  
713-15  
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

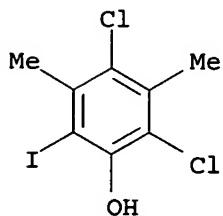
AB The reagent (dichloramine-T and NaI) was added cautiously to a well-stirred solution of the phenol or ether in HOAc at room temperature, except for hydroxy and alkoxynaphthoic acids which reacted at 60-75°. With exception of o- and p-C<sub>6</sub>H<sub>4</sub>(OMe)<sub>2</sub>, the yields were 75-92%. Below are listed the products (and their m.ps.) obtained by this method: p-IC<sub>6</sub>H<sub>4</sub>OMe, 52°; p-IC<sub>6</sub>H<sub>4</sub>OEt, 27°; 1,2-IC<sub>10</sub>H<sub>6</sub>OMe, 88°; 1,2-IC<sub>10</sub>H<sub>6</sub>OEt, 74°; 4,1-IC<sub>10</sub>H<sub>6</sub>OEt, 45°; 6,2,4-ICl<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OH, 62°; 6,2,4-IBr<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OH, 104°; 5-iodo-3-nitro-p-cresol, 83°; 2-chloro-4-iodo-m-5-xyleneol, 90°; 2-chloro-4,6-diiodo-m-5-xyleneol, 131°; 2,4-dichloro-6-iodo-m-5-xyleneol, 130°; 3,5-diiodosalicylic acid, 233°; 4-hydroxy-3,5-diiodobenzoic acid,

262°; 3-hydroxy-4-iodo-2-naphthoic acid, 210° (decomposition);  
 6-hydroxy-5-iodo-2-naphthoic acid, 234°; 5-iodo-6-methoxy-2-naphthoic acid, 292° (decomposition); 5-iodo-6-lauroyloxy-2-naphthoic acid, mesomorphic, smectic phase 145-67°, nematic phase 167-70°; 8-iodo-7-octyloxy-2-naphthoic acid, 148°; 7-cetyloxy-8-iodo-2-naphthoic acid, 123°; 4,6-diiodo-1,3-dimethoxybenzene, 75°; 4,5-diiodo-1,2-dimethoxybenzene, 134° (30% yield); 2,5-diiodo-1,4-dimethoxybenzene, 171° (20% yield); 2,4-diiodo-3,5-dimethoxybenzene, 125° (50% yield).

IT 791626-88-5, 3,5-Xylenol, 2,4-dichloro-6-iodo- 791626-94-3  
 , 3,5-Xylenol, 4-chloro-2,6-diiodo-  
 (preparation of)

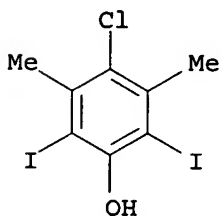
RN 791626-88-5 CAPLUS

CN 3,5-Xylenol, 2,4-dichloro-6-iodo- (5CI) (CA INDEX NAME)



RN 791626-94-3 CAPLUS

CN 3,5-Xylenol, 4-chloro-2,6-diiodo- (5CI) (CA INDEX NAME)



L11 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1950:34747 CAPLUS  
 DOCUMENT NUMBER: 44:34747  
 ORIGINAL REFERENCE NO.: 44:6645h-i,6646a-e  
 TITLE: Halogenated anthraquinone dyes  
 PATENT ASSIGNEE(S): Sandoz Ltd.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

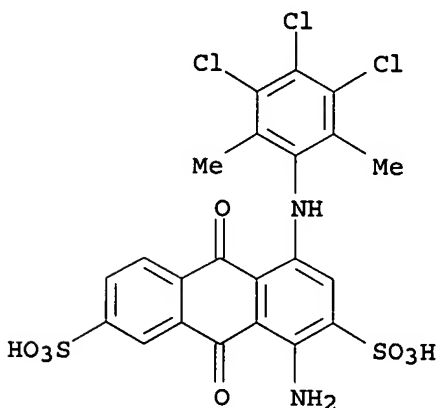
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 259730		19490701	CH	

AB Halogenation of 1-amino-4-anilinoanthraquinonedisulfonic acids is described. The products dye wool, silk, and nylon in bright reddish blue shades. K 1-amino-4-(2,4,6-trimethylanilino)-2,6-anthraquinonedisulfonate (I) 5.9 g. is dissolved at 25° in 85% H<sub>2</sub>SO<sub>4</sub> 50 and chlorinated at 20-30° with Cl<sub>2</sub>. The mixture is heated 1 h. at 60° and drowned in ice and H<sub>2</sub>O to obtain the reddish blue crystals of H<sub>2</sub>O-soluble dye, 1-amino-4-(3,5-dichloro-2,4,6-trimethylanilo)-2,6-anthraquinonedisulfonic acid. In Swiss 259,731, K 1-amino-4-(2,6-dimethylanilino)-2,8-anthraquinonedisulfonate 5.8 is brominated in 90% H<sub>2</sub>SO<sub>4</sub> 50 with Br 1.8 at 40° for 3 h. to give 1-amino-4-(dibromo-2,6-dimethylanilino)-2,8-anthroquinonedisulfonic acid. In Swiss 259,732, Na 1-amino-4-(2,6-diethylanilino)-2,7-anthraquinonedisulfonate, brominated as above at 60° for 3 h. gave 1-amino-4-(dibromo-2,6-di-ethylanilino)-2,7-anthraquinonedisulfonic acid. In Swiss 259,733, Na



1-amino-4-(2',4',6-trimethylanilino)-2,5-anthraquinonedisulfonate 5.6 is brominated in 100% H2SO4 30 with Br 1.8 by stirring at 20-30° overnight and heating if necessary to 100° for completion. The crystals of 1-amino-4-(3,5-dibromo-2,4,6-trimethylanilino)-2,5-anthraquinonedisulfonic acid (II) are reddish blue. In Swiss 259,734, I 5.9 is brominated in 90% H2SO4 30 by stirring overnight at 20-30° and heating as required to 100° for completion to give the 2,6-isomer of II. In Swiss 259,735, Na 1-amino-4-(2,4,6-triethylanilino)-2,8-anthraquinonedisulfonate 6 is brominated in 100% H2SO4 30 with Br 1.8 at 20-30° and then heated if necessary to 60° for completion to give 1-amino-4-(3,5-dibromo-2,4,6-triethylanilino)-2,8-anthraquinonedisulfonic acid (III). In Swiss 259,736, 1-amino-2-bromo-4-(2,6-dimethyl-4-chloroanilino)-7-anthraquinonesulfonic acid 5 in 1-2% oleum 25 is treated with iodine 0.05 and Cl 2. The dye is isolated as before and converted to the 2,7-disulfonic acid by replacement of the -Br with -SO3H using K2SO3 under pressure. The dye is 1-amino-4-(3,4,5-trichloro-2,6-dimethylanilino)-2,7-anthraquinonedisulfonic acid. In Swiss 259,737, Na 1-amino-2-bromo-4-(2,4,6-triethylanilino)-6-anthraquinonesulfonate 5.8 is brominated in 90% H2SO4 30 with Br 2. After stirring overnight at 20-30° the temperature is raised to 100° for 1-2 h. for completion. This dye is converted as above to the disulfonate using K2SO3 under pressure to give the 2,6-isomer of III. In Swiss 259,738, Na 1-amino-4-(2,3,6-triethylanilino)-2,5-anthraquinonedisulfonate is brominated at 40° for 3 h. in 95% H2SO4 50 with Br 1. 1-Amino-4-(bromo-2,3,6-triethylanilino)-2,5-anthraquinonedisulfonic acid is obtained in the form of reddish-blue needles.

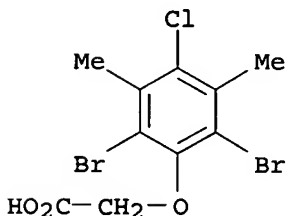
IT 737803-95-1, 2,7-Anthraquinonedisulfonic acid,  
1-amino-4-(3,4,5-trichloro-2,6-xylylidino)-  
(preparation of)  
RN 737803-95-1 CAPLUS  
CN 2,7-Anthraquinonedisulfonic acid, 1-amino-4-(3,4,5-trichloro-2,6-xylylidino)-  
(5CI) (CA INDEX NAME)



L11 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1948:38890 CAPLUS  
DOCUMENT NUMBER: 42:38890  
ORIGINAL REFERENCE NO.: 42:8255e-i  
TITLE: The effect of Tween 80 in vitro on the bacteriostatic activity of twenty compounds for Mycobacterium tuberculosis  
AUTHOR(S): Youmans, Anne S.; Youmans, Guy P.  
CORPORATE SOURCE: Northwestern Univ. Med. School, Chicago  
SOURCE: Journal of Bacteriology (1948), 56, 245-52  
CODEN: JOBAAAY; ISSN: 0021-9193  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB Unpurified Tween 80 in a synthetic medium, as compared to the medium alone, increased the activity of the following compds.: sulfanilamide; sulfapyridine; sulfathiazole; 4-allylaminophenyl 4-aminophenyl sulfone;

2-nitro-5-sulfanilylthiophene; di(2-nitro-5-thienyl) sulfone; di(4-aminophenyl) sulfone; p-xyloquinone; 1,4-naphthoquinone; 2-chloro-1,4-naphthoquinone; 8-hydroxyquinoline; (2,6-dibromo-3,5-dimethyl-4-chlorophenoxy)acetic acid; 4-amino-2-hydroxybenzoic acid-HCl; 3-indolepropionic acid; and chloromycetin. It decreased the activity of: p-aminoazobenzene; 2-(4-aminophenyl)pyridine; and 4-chlorophenyl 4-aminophenyl sulfide. It had no effect on: 2-methylnaphthoquinone and N-(p-aminophenyl)piperidine. Crystalline bovine albumin increased the activity of 13 out of the 20 compds. If Tween and albumin were both present; 5 compds. were more bacteriostatic, 4 gave approx. the same results as the basal medium, and 11 were less bacteriostatic. Purified Tween had less effect than unpurified Tween. Decreasing the concentration of Tween by 4-fold did not alter significantly the bacteriostatic levels of 5 compds. studied. The free oleic acid which may be present in Tween apparently was not responsible for the effect of Tween on the bacteriostatic activities of the compds. mentioned. 17 references.

IT 764710-09-0, Acetic acid, (2,6-dibromo-4-chloro-3,5-xilyloxy) -  
(bacteriostatic activity for Mycobacterium tuberculosis)  
RN 764710-09-0 CAPLUS  
CN Acetic acid, (2,6-dibromo-4-chloro-3,5-dimethylphenoxy) - (9CI) (CA INDEX NAME)



L11 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1948:23164 CAPLUS

DOCUMENT NUMBER: 42:23164

ORIGINAL REFERENCE NO.: 42:4957h-i,4958a-e

TITLE: Halogenation of m-5- and m-2-xilenols. Preparation and structure of certain polyhalo-m-5- and -m-2-xilenols

AUTHOR(S): Elston, C. H. R.; Peters, A. T.; Rowe, F. M.

CORPORATE SOURCE: Univ. of Leeds, UK

SOURCE: Journal of the Chemical Society (1948)  
367-70

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

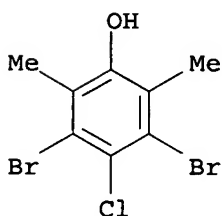
AB 2,4,6-Br<sub>3</sub>C<sub>6</sub>H<sub>2</sub>OH (I) (16 g. as a paste with 20 cc. H<sub>2</sub>O), treated with 16 g. Cl in 2000 cc. H<sub>2</sub>O at room temperature, gives 2,4,6-tribromophenol chloride (II), yellow, m. 125-30° (decomposition); the alc. solution of II, decolorized with SO<sub>2</sub>, gives a mixture of I and 4,2,6-ClBr<sub>2</sub>C<sub>6</sub>H<sub>2</sub>OH (III). III (14.3 g.) and 8.8 g. Br in dilute AcOH give 4-chloro-2,6-dibromophenol bromide, pale yellow, m. 99-100°, decompose 120°; SO<sub>2</sub> in EtOH gives only III. 2,4,6,3,5-Br<sub>3</sub>Me<sub>2</sub>C<sub>6</sub>OH (IV) in AcOH, treated with 1 mol. Cl below 30°, the solution poured into H<sub>2</sub>O, the wet product taken up in petr. ether at 30-40°, and the residue quickly crystallized from petr. ether, gives 2-chloro-2,4,6-tribromo-1,3-dimethyl-3,6-cyclohexadien-5-one, m. 120-2°; decomposition with SO<sub>2</sub> yields mainly 2,4,6,3,5-ClBr<sub>2</sub>Me<sub>2</sub>C<sub>6</sub>OH (V); the action of 2.5 mols. Cl on V in AcOH at 10° and the mixture allowed to stand overnight gives 2,2,4-trichloro-6-bromo-1,3-dimethyl-3,6-cyclohexadien-5-one, very pale yellow, m. 105°, moderately stable when dry but the crude product decompose readily; SO<sub>2</sub> in EtOH gives 2,6,4,3,5-Cl<sub>2</sub>BrMe<sub>2</sub>C<sub>6</sub>OH, m. 165-6°. Br does not react with V but with 2,4,6,3,5-Cl<sub>3</sub>Me<sub>2</sub>C<sub>6</sub>OH (VI) in AcOH at 60° (with heating 2 min. at 110° and standing overnight at room temperature) it yields 2,4,6-trichloro-3,5-xylene bromide, yellow, m. 112°; it decompose rapidly in air and on boiling with EtOK it gives VI. 4,6,2,3,5-Cl<sub>2</sub>BrMe<sub>2</sub>C<sub>6</sub>OH in AcOH, treated at 40-50° with 1.2 mols. Cl, gives about 4 parts 2,2,4,6-tetrachloro-1,3-dimethyl-3,6-cyclohexadien-5-one

(VIA) (m. 107-8°) and 1 part of a compound m. 106-7° (mixed m.p. 70-90°), stable to SO<sub>2</sub> in aqueous EtOH, whose constitution was not established. 2,6,3,4,5-Me<sub>2</sub>Br<sub>3</sub>C<sub>6</sub>OH (VII) and 2 mols. Br in H<sub>2</sub>O give 85.3% 3,4,5-tribromo-2,6-xyleneol bromide (VIII), yellow, m. 139-40°; decomposition of VIII with boiling EtOH (more readily with SO<sub>2</sub> in EtOH) gives VII; Zn and H<sub>2</sub>O gives VII and some 4,5-di-Br derivative; boiling aqueous KI gives scarlet needles, m. 156-8°, of the adduct of 1 mol. 4,6-dibromo-m-xyloquinone and 2 mols. VIII. VII and 2.1 mols. Cl in AcOH, warmed 2 min. at 60° and kept 2 hrs. at room temperature, give 3,4,5-tribromo-2,6-xyleneol chloride, yellow, m. 60-1°; prolonged boiling with EtOH gives VII. The only products isolated from 4,3,5,2,6-ClBr<sub>2</sub>Me<sub>2</sub>C<sub>6</sub>OH (IX) and Br were 4,6-dibromo-m-xyloquinone (X) and an adduct of 1 mol. X and 2 mols. IX, m. 138-40°. Absorption spectra are given for PhOH, VI, VIA, C<sub>6</sub>H<sub>4</sub>O<sub>2</sub>, tetrabromo-2,6-xyleneol, and II; the data support the quinonoid structure of the polyhalo compds.

IT 857974-71-1, 2,6-Xyleneol, 3,5-dibromo-4-chloro-, compound with 3,5-dibromo-m-xyloquinone 859783-89-4, 3,5-Xyleneol, 2,4,6-trichloro-, hypobromite 874519-00-3, 3,5-Xyleneol, 2-bromo-4,6-dichloro-  
(preparation of)  
RN 857974-71-1 CAPLUS  
CN m-Xyloquinone, 3,5-dibromo-, compd. with 3,5-dibromo-4-chloro-2,6-xyleneol (5CI) (CA INDEX NAME)

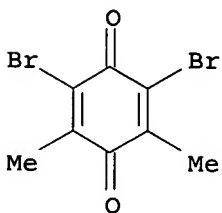
CM 1

CRN 408326-71-6  
CMF C8 H7 Br2 Cl O



CM 2

CRN 87405-27-4  
CMF C8 H6 Br2 O2



RN 859783-89-4 CAPLUS  
CN 3,5-Xyleneol, 2,4,6-trichloro-, hypobromite (5CI) (CA INDEX NAME)

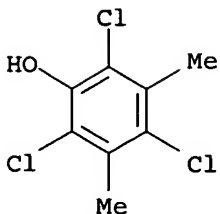
CM 1

CRN 13517-11-8  
CMF Br H O

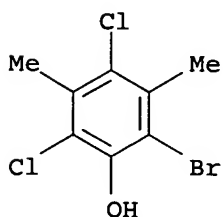
Br—OH

CM 2

CRN 6972-47-0  
CMF C8 H7 Cl3 O



RN 874519-00-3 CAPLUS  
CN 3,5-Xylenol, 2-bromo-4,6-dichloro- (5CI) (CA INDEX NAME)



L11 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1948:21313 CAPLUS

DOCUMENT NUMBER: 42:21313

ORIGINAL REFERENCE NO.: 42:4548h-i,4549a-d

TITLE: Halogenation of 3,5- and 2,6-xylenol. Mixed chlorobromo derivatives

AUTHOR(S): Gleed, S. W.; Peters, A. T.

CORPORATE SOURCE: Univ. Leeds, UK

SOURCE: Journal of the Chemical Society (1948)  
209-11

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

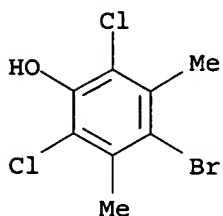
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 42:21313

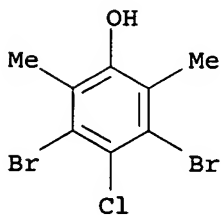
AB 1,3,2,5-Me2ClC6H2OH (I) (20 g.) in 200 cc. CHCl3 containing a little anhydrous AlBr3, treated rapidly with 20.5 g. Br in 100 cc. CHCl3, gives 96.3% 4-chloro-2-bromo-3,5-xylenol (II), m. 68°. 1,3,2,5-Me2BrC6H2OH (III) (20 g.) in CHCl3 containing a little iodine, treated rapidly with 7.1 g. Cl in 100 cc. CHCl3, gives 77-4% 2-chloro-4-bromo-3,5-xylenol (IV), m. 90-110°. I (50 g.) in 600 cc. AcOH with 103 g. Br in 200 cc. AcOH (3 hrs.) gives 87.5% 1,3,4,6,2-Me2Br2ClC6OH, m. 164° (cf. Lesser and Gad, C.A. 17, 3181). IV with an addnl. mol. of Cl gives a nearly quant. yield of 2,6-dichloro-4-bromo-3,5-xylenol, m. 182°; in larger quantities, it was prepared in 87% yield by slowly adding 37 g. Cl in 500 cc. AcOH to 52 g. III in 500 cc. cold AcOH. II (15 g.) in 120 cc. AcOH, treated (below 20°) with 4.5 g. Cl in 150 cc. AcOH, gives 97.6% 4,6-dichloro-2-bromo-3,5-xylenol (V), m. 165-6°; V results in 84.7% yield by slowly adding 10 g. Br in 80 cc. AcOH to 12 g. 1,3,2,4,5-Me2Cl2C6HOH in 120 cc. AcOH at room temperature. Oxidation of V at 100° with HNO3 (d. 1.42) gives 5-chloro-3-bromo-m-xyloquinone (VI), yellow, m. 170-1°. IV (14.7 g.) and 10 g. Br in AcOH (temperature below 20°) give 90% 6-chloro-2,4-dibromo-3,5-xylenol, m. 170°; oxidation gives VI. 1,3,5,2-Me2ClC6H2OH (VII) (15 g.) in 150 cc. CHCl3 containing a little AlBr3, treated rapidly with 16.8 g. Br in 75 cc. CHCl3 and the mixture kept 2 hrs. at 50°, give 96.6% 4-chloro-3-bromo-2,6-xylenol (VIII), m. 86-7°. Molten VIII (2.3 g.), added (15 min.) to 7.4 g. liquid Br at room temperature, gives 96.9% 4-chloro-3,5-dibromo-2,6-

xilenol (IX), m. 188-9°; addition of 2 mols. Br in 12 times its weight of H2O to finely ground IX at room temperature gives 3,5-dibromo-m-xyloquinone (X) and a scarlet adduct of 1 mol. X and 2 mols. IX, m. 141-2° (also prepared from the 2 components). IX is prepared in 98.5% yield by gradual addition of 1 mol. VII to 4 mols. liquid Br (1 hr.) at 20°. Addition of 5.75g. molten 1,3,4,5,2-Me2Cl2C6HOH to 19.3 g. Br at room temperature gives 98.4% 4,5-dichloro-3-bromo-2,6-xilenol, pale yellow, m. 188°. Improved directions are given for the preparation of the 4-Br, 3,4-di-Br, and 3,4,5-tri-Br derivs. of 2,6-Me2C6H3OH.

IT 408314-44-3, 3,5-Xylenol, 4-bromo-2,6-dichloro-  
 408326-71-6, 2,6-Xylenol, 3,5-dibromo-4-chloro-  
 857974-71-1, m-Xyloquinone, 3,5-dibromo-, compound with  
 3,5-dibromo-4-chloro-2,6-xilenol 859784-53-5, 3,5-Xylenol,  
 2,4-dibromo-6-chloro- 874519-00-3, 3,5-Xylenol,  
 2-bromo-4,6-dichloro-  
 (preparation of)  
 RN 408314-44-3 CAPLUS  
 CN Phenol, 4-bromo-2,6-dichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



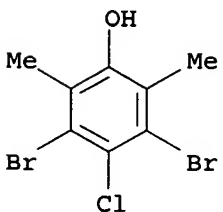
RN 408326-71-6 CAPLUS  
 CN Phenol, 3,5-dibromo-4-chloro-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 857974-71-1 CAPLUS  
 CN m-Xyloquinone, 3,5-dibromo-, compd. with 3,5-dibromo-4-chloro-2,6-xilenol  
 (5CI) (CA INDEX NAME)

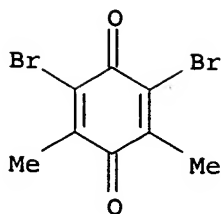
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CRN 408326-71-6  
 CMF C8 H7 Br2 Cl O

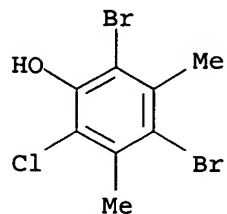


CM 2

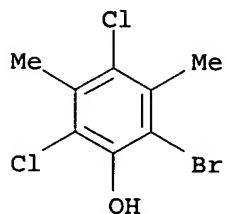
CRN 87405-27-4  
 CMF C8 H6 Br2 O2



RN 859784-53-5 CAPLUS  
CN 3,5-Xylenol, 2,4-dibromo-6-chloro- (5CI) (CA INDEX NAME)



RN 874519-00-3 CAPLUS  
CN 3,5-Xylenol, 2-bromo-4,6-dichloro- (5CI) (CA INDEX NAME)



L11 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1946:4859 CAPLUS

DOCUMENT NUMBER: 40:4859

ORIGINAL REFERENCE NO.: 40:782h-i,783a-c

TITLE: Melting points and unit cells of the methylbenzenes

AUTHOR(S): Beacall, T.

SOURCE: Transactions of the Faraday Society (1945),  
41, 472-9

CODEN: TFSOA4; ISSN: 0014-7672

DOCUMENT TYPE: Journal

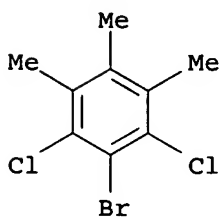
LANGUAGE: Unavailable

AB cf. C.A. 38, 671.6. M.ps. of the 12 possible Me derivs. of benzene and of the following 30 halogen derivs. are related to the dimensions of the unit cells as determined from available x-ray analyses: pentabromotoluene, pentachlorotoluene, 6-chloro-2,3,4,5-tetrabromotoluene, 2,3,5,6-tetrachloro-4-bromotoluene, tetrabromo derivs. of o-, m-, and p-xylenes, tetrachloro derivs. of o-, m-, and p-xylenes, 6-chloro-2,3,5-tribromo-p-xylene, 3,6-dichloro-2,5-dibromo-p-xylene, 3,5,6-trichloro-2-bromo-p-xylene, 4,6-dichloro-3,5-dibromo-o-xylene, 4,6-dichloro-2,5-dibromo-m-xylene, 2,6-dichloro-4,5-dibromo-m-xylene, 2,4,6-tribromo-1,3,5-trimethylbenzene, 3,5,6-tribromo-1,2,4-trimethylbenzene, 4,5,6-tribromo-1,2,3-trimethylbenzene, 2,4,6-trichloro-1,3,5-trimethylbenzene, 3,5,6-trichloro-1,2,4-trimethylbenzene, 4,5,6-trichloro-1,2,3-trimethylbenzene, 4,6-dichloro-5-bromo-1,2,3-trimethylbenzene, 3,6-dibromo-1,2,4,5-tetramethylbenzene, 4,6-dibromo-1,2,3,5-tetramethylbenzene, 5,6-dibromo-1,2,3,4-tetramethylbenzene, 3,6-dichloro-1,2,4,5-tetramethylbenzene, 5,6-dichloro-1,2,3,4-tetramethylbenzene,

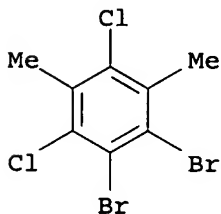
bromopentamethylbenzene, chloropentamethylbenzene. The m.ps. of p-xylene, durene, and hexamethylbenzene form a geometrical series; the vols. of the unit cell per mol. approx. to an arithmetical series. It is suggested that in these mols. the pairs of Me groups in para position are linked to Me groups of adjacent mols. The volume of the unit cell of pentabromotoluene as determined from its mol. weight and d. is in agreement with that of benzene plus increments due to the 3 pairs of substituents. The lowering in m.p. by introduction of a single Me group points to a head-to-tail linkage in the unit cell. A tentative structure for the unit cell of mesitylene is suggested after the low m.p. of mesitylene is contrasted with the comparatively high m.p. of the sym. trihalobenzenes.

IT 679427-57-7, Hemimellitene, 5-bromo-4,6-dichloro-  
 679428-36-5, m-Xylene, 4,5-dibromo-2,6-dichloro-  
 679428-38-7, m-Xylene, 2,5-dibromo-4,6-dichloro-  
 679428-39-8, p-Xylene, 2,3,5-tribromo-6-chloro-  
 679428-40-1, o-Xylene, 3,5-dibromo-4,6-dichloro-  
 679428-41-2, p-Xylene, 2-bromo-3,5,6-trichloro-  
 (m.p. and unit cell of)

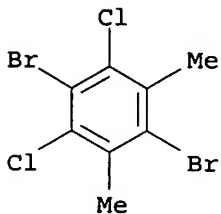
RN 679427-57-7 CAPLUS  
 CN Hemimellitene, 5-bromo-4,6-dichloro- (4CI) (CA INDEX NAME)



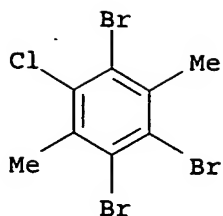
RN 679428-36-5 CAPLUS  
 CN m-Xylene, 4,5-dibromo-2,6-dichloro- (4CI) (CA INDEX NAME)



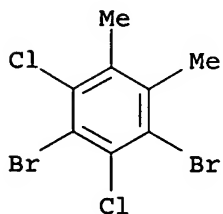
RN 679428-38-7 CAPLUS  
 CN m-Xylene, 2,5-dibromo-4,6-dichloro- (4CI) (CA INDEX NAME)



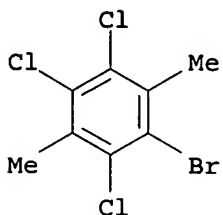
RN 679428-39-8 CAPLUS  
 CN p-Xylene, 2,3,5-tribromo-6-chloro- (4CI) (CA INDEX NAME)



RN 679428-40-1 CAPLUS  
 CN o-Xylene, 3,5-dibromo-4,6-dichloro- (4CI) (CA INDEX NAME)



RN 679428-41-2 CAPLUS  
 CN p-Xylene, 2-bromo-3,5,6-trichloro- (4CI) (CA INDEX NAME)



L11 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1945:29888 CAPLUS

DOCUMENT NUMBER: 39:29888

ORIGINAL REFERENCE NO.: 39:4855i,4856a-i

TITLE: Synthesis and antitubercular studies of halogenated phenyl ethers

AUTHOR(S): Burger, Alfred; Wilson, Elizabeth L.; Brindley, C. O.; Bernheim, Frederick

SOURCE: Journal of the American Chemical Society (1945), 67, 1416-19

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

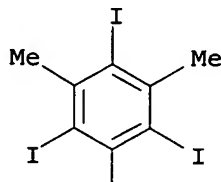
LANGUAGE: Unavailable

AB In general, 100 g. of the phenol in a mixture of 800 cc. 20% NH<sub>4</sub>OH and 200 to 800 cc. MeOH was treated with the calculated amount of iodine solution (containing 1 part of iodine and 2 parts KI in 4 parts of H<sub>2</sub>O) at such a rate that the brown color never persisted for any length of time; the crude yields were above 90% but 5-20% was lost during purification; the anisoles were prepared from the Na phenolates and Me<sub>2</sub>SO<sub>4</sub> and the lauryl ethers from the Na salts and lauryl iodide in MeOH. 2,6-Diiodo-4-chloroanisole, m. 65°; 2,4,6-triiodo-1-dodecoxybenzene (I), m. 63-4°; 3-Me derivative (II), m. 47-8°; 2,4,6-triiodo-3,5-dimethylphenol, m. 175-7° (decomposition); 2,4-diiodo-4-tert-amylphenol, m. 62°; 2-bromo-4-phenyl-6-iodophenol, m. 86.5-8°; 2,4-diiodo-4-tert-butylphenol, m. 82°. Most of the basic ethers were prepared from 0.1 mole of the phenol in 0.2 mole of Na in MeOH at 30-50° and 0.12 mole of a dialkylaminoalkyl chloride-HCl on refluxing 5 to 12 hrs.; 0.1 mole of NaI was added as a catalyst; the yields averaged 25 to 35%; with Me<sub>2</sub>N(CH<sub>2</sub>)<sub>2</sub>Cl the yield was sometimes below 5%; dialkylaminopropyl chlorides gave from 50 to 90% yields. Ethers of 2,4,6-I<sub>3</sub>C<sub>6</sub>H<sub>2</sub>OH (HCl salts



in all cases unless stated): 2-dimethylaminoethyl, m. 226° (decomposition); 2-dibutylaminoethyl, m. 192-4° (decomposition); 2-morpholinoethyl, m. 240-2° (decomposition) (free base, m. 130-1°); 3-diethylaminopropyl, m. 190-2° (decomposition). 2,6,4-I2BrC6H2OH: 2-diethylaminoethyl, m. 174-7° (decomposition). 2,6,4-I2ClC6H2OH: 2-diethylaminoethyl, m. 182° (decomposition); 3-diethylaminopropyl, m. 214° (decomposition). 2,4,6-I2ClC6H2OH: diethylaminoethyl, m. 155-6°; 3-(2-methylpiperidino)propyl, m. 188° (decomposition). 2,6,4-I2PhC6H2OH: 2-diethylaminoethyl, m. 198-9° (decomposition). 2,6,4-I2MeC6H2OH: 2-diethylaminoethyl, m. 166.5°. 2,4,6-I2MeC6H2OH: 2-diethylaminoethyl, m. 151-2°. 2,4,6,3-I3MeC6HOH: 2-diethylaminoethyl, m. 173-4°; 2-dibutylaminoethyl, m. 190-3° (decomposition). 2,4,6,3,5-I3Me2C6OH: 2-diethylaminoethyl, m. 209° (decomposition). 2,6,4-IBrPhC6H2OH: 2-diethylaminoethyl, m. 190-1° (decomposition). 2,6-Diiodo-4-phenylazophenol: 2-diethylaminoethyl, m. 188-90° (decomposition). 2,4,6-Br3C6H2OH: 2-dimethylaminoethyl, m. 194°; 2-diethylaminoethyl, m. 149°. 2,4,6-Cl3C6H2OH: 2-dimethylaminoethyl (free base), b4 131-3° (picrate, m. 192-3°); 2-diethylaminoethyl, m. 160-2°; 3-(2-methylpiperidino)propyl, m. 156-7°. 2,4,5-Cl3C6H2OH: diethylaminomethyl, m. 157-9° (decomposition); 2-dimethylaminoethyl, m. 210-11°; 2-diethylaminoethyl, m. 183°; 2-dibutylaminoethyl, m. 124°; 3-diethylaminopropyl, m. 179°; 3-dibutylaminopropyl (free base), b2 180-90° (picrate, m. 119-20°); 3-(2-methylpiperidino)propyl, m. 229-30°; 2-butylaminoethyl, m. 122°. 2,4-Cl2C6H3OH: 2-dibutylaminoethyl, m. 295-7°. Cl5C6OH: 3-(2-methylpiperidino)propyl, m. 224° (decomposition). PhOH: 2-diethylaminoethyl, m. 137.5°. 4-tert-BuC6H4OH: 2-diethylaminoethyl, m. 158-60°. 4-tert-AmC6H4OH: 2-diethylaminoethyl, m. 128-31°. 3-Me2C6H3OH: 2-dibutylaminoethyl (free base), b1 147-50°. 3,5-Me2C6H3OH: 2-diethylaminoethyl, m. 132°. In general, chemotherapeutic activity was not restricted to compds. containing aliphatic NH2 groups; the ethers containing the 3-(2-methylpiperidino)propyl radical were highly active. Activity, but also toxicity in guinea pigs, was usually greater in dialkylaminopropyl than in the corresponding dialkylaminoethyl ethers; shortening of the ethylene group, in a trihalophenoxy(diethylamino)methane derivative, caused complete loss of antitubercular action. Replacement of the Bu2N group in an active ether by the BuNH group also abolished activity. Replacement of nuclear iodine by other halogens did not lead to a definite pattern correlating chemical structure to antitubercular activity. Nuclear Br had a slightly dystherapeutic effect, whereas several of the poly-Cl derivs. rivaled analogous iodinated compds. Nuclear iodine does not appear superior to other halogens in the tuberculostatic activity of this series. I and II has no activity, probably because of the insoly. of these ethers in polar solvents.

IT 854640-87-2, Triethylamine, 2-(2,4,6-triiodo-3,5-xylyloxy)-, hydrochloride (preparation of)  
 RN 854640-87-2 CAPLUS  
 CN Triethylamine, 2-(2,4,6-triiodo-3,5-xylyloxy)-, hydrochloride (4CI) (CA INDEX NAME)



ACCESSION NUMBER: 1938:41756 CAPLUS  
DOCUMENT NUMBER: 32:41756  
ORIGINAL REFERENCE NO.: 32:5802h-i,5803a-f  
TITLE: Aristols. Preparation and constitution of aristols  
derived from p-xylene and sym-m-xylene. II  
AUTHOR(S): Bordeianu, C. V.  
SOURCE: Annales Scientifiques de l'Universite de Jassy (1937), 23(Pt. I), 240-64  
CODEN: ASUJAH; ISSN: 0365-7264

DOCUMENT TYPE: Journal

LANGUAGE: French

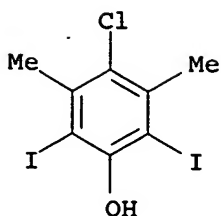
GI For diagram(s), see printed CA Issue.

AB By direct mercuriation of the corresponding halogen-substituted xylene (cf. preceding abstrs.) the following compds. were prepared:  
2,5-dimethyl-4-bromo-6-acetoxymercuriphenol (I), 91% yield;  
2,5-dimethyl-4-iodo-6-acetoxymercuriphenol (II), 80-90% yield;  
3,5-dimethyl-4-bromo-6-acetoxymercuriphenol (III), almost quant. yield;  
3,5-dimethyl-4-chloro-6-acetoxymercuriphenol (IV); and  
3,5-dimethyl-4-chloro-5-iodo-2-acetoxymercuriphenol (V). All were insol. in H<sub>2</sub>O, soluble in glacial AcOH and soluble without decomposition in NaOH. Treated with CO<sub>2</sub> in the presence of alkali, they gave the internal Hg oxides (cf. Bordeianu, loc. cit.) and with NaI and I (Dimroth's reaction) gave iodides in which the I replaced the AcOHg group. Thus, I gave 90% of 2,5-dimethyl-4-bromo-6-iodophenol (VI), m. 64-5° (from petr. ether); acetate, m. 73° (from glacial AcOH). II yielded 2,5-dimethyl-4,6-diiodophenol (VII), m. 63° (from glacial AcOH), identical with the compound previously reported (C. A. 30, 1760.5) which is oxidized by K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in AcOH to give 60% of a quinone (from analogy with iodothymoquinone, presumably of the structure CO.CMe:CI.CO.CMe:CH), m. 79-80° (from 60-70% alc.), deep orange, sublimes and steam-distills (monooxime yellow, insol. in H<sub>2</sub>O, decomp. 170°; dioxime could not be prepared). III yielded 3,5-dimethyl-4-bromo-6-iodophenol (VIII), m. 85.5° (from petr. ether). IV gave 3,5-dimethyl-4-chloro-6-iodophenol (IX), colorless, m. 92-3° (from petr. ether); acetate, m. 86° (from alc.). V gave 100% of 3,5-dimethyl-2,6-diiodo-4-chlorophenol (X), colorless, m. 131-2° (from alc., Et<sub>2</sub>O or AcOH), which can be prepared also from 3,5-dimethyl-4-chlorophenol with I and alkali (poor yields) or with I and NH<sub>3</sub> in MeOH; acetate, m. 147-8° (from glacial AcOH). Compds. VI-X are colorless and soluble in dilute alkalies. Oxidizing agents in alkaline media convert the dihalides to aristols, insol. in alkalies; e.g., VI and VII with K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and KOH or with I and KOH give quant. yields of the aristol 5,5'-diiodo-3,6,3',6'-dimethyl-4,4'-biphenylquinone (CH:CMe.CO.CI:CMe.C):2, also made by the action of alkali on p-xylene. Similarly the aristol 3,5,3',5'-tetraiodo-2,6,2',6'-tetramethyl-4,4'-biphenylquinone (XI) is prepared in quant. yields from X, from 2,3,5-triiodo-3,5-dimethylphenol (XII) and from 2,6-diiodo-4-bromo-3,5-dimethylphenol (XIII). The reasons for assigning the particular structures are similar to those set forth in C. A. 28, 2339.1, and the fact that Br from XIII is recovered quant. as the bromate. The mol.-weight determination on XI gave values twice as great as required by the formula assigned, so the substance must actually exist as a dimer. B. claims that while the preparation of XII was described in the article abstracted in C. A. 30, 1760.5, it was called (incorrectly) the diiodide-the data on mol. weight and % I were for the diiodide, but the properties and preparation were for the triiodide (XII), whose purification is described in detail in the present article. XIII is synthesized directly from I and 4-bromo-3,5-dimethylphenol, only if 5 mols. of NaOH and 4 mols. of I are used for each mol. of XIV. If less I is employed, XII is precipitated. The aristol which is mentioned as being formed from IX is not described.

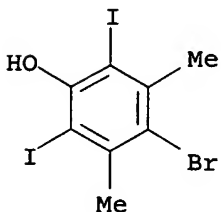
IT 791626-94-3, 3,5-Xylene, 4-chloro-2,6-diiodo- 854672-30-3  
, 3,5-Xylene, 4-bromo-2,6-diiodo- 856351-96-7, 3,5-Xylene,  
4-chloro-2,6-diiodo-, acetate  
(preparation of)

RN 791626-94-3 CAPLUS

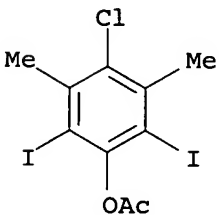
CN 3,5-Xylene, 4-chloro-2,6-diiodo- (5CI) (CA INDEX NAME)



RN 854672-30-3 CAPLUS  
CN 3,5-Xylenol, 4-bromo-2,6-diiodo- (4CI) (CA INDEX NAME)



RN 856351-96-7 CAPLUS  
CN 3,5-Xylenol, 4-chloro-2,6-diiodo-, acetate (4CI) (CA INDEX NAME)



L11 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1937:56695 CAPLUS

DOCUMENT NUMBER: 31:56695

ORIGINAL REFERENCE NO.: 31:7856i,7857a-c

TITLE: 3,5-Dibromo-p-xylydine; 3,5,6-tribromo-p-xylydine and some of their derivatives

AUTHOR(S): Bures, E.; Meskan, F.

SOURCE: Casopis Ceskoslovenskeho Lekarnictva (1937), 17, 149-60

CODEN: CCLEA3

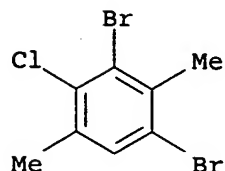
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

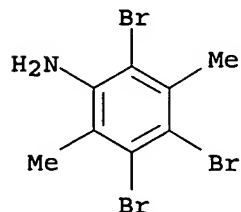
AB The bromination of an alc. solution of p-xylydine, at room temperature and without an access to sunlight, resulted in the formation of 3,5-dibromo-p-xylydine. The constitution of this compound was proved by its transformation into 2,3,5-tribromo-p-xylenol. From 3,5-dibromo-p-xylydine there were prepared the following derivs.: 3,5-dibromo-p-acetxylydine, b. 163°; 3,5-dibromo-p-diacetxylydine, b. 56°; 3,5-dibromo-p-benzoylxylydine, b. 192°; 3,5-dibromo-p-xylene, b. 36°; 3,5-dibromo-2-chloro-p-xylene, b. 85°; 2,3,5-tribromo-p-xylene, b. 89°; 1,4-dimethyl-3,5-di-bromo-2-benzonitrile, b. 97°, and 3,5-dibromo-p-xylenol, b. 82°. From this last compound there were prepared the Hg and Bi xylenolates and its Me ether. By the careful bromination of the diluted solution of p-acetxylydine in glacial AcOH, there was obtained 3,5,6-tribromo-1,4-dimethyl-2-acetaminobenzene.

IT 854662-93-4, p-Xylene, 3,5-dibromo-2-chloro- 854673-69-1  
, 2,5-Xylydine, 3,4,6-tribromo- 856356-94-0, 2,5-Acetoxylide,  
3,4,6-tribromo-  
(preparation of)

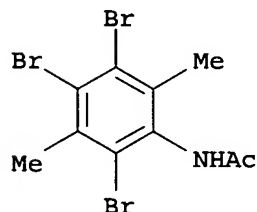
RN 854662-93-4 CAPLUS  
CN p-Xylene, 3,5-dibromo-2-chloro- (4CI) (CA INDEX NAME)



RN 854673-69-1 CAPLUS  
CN 2,5-Xylidine, 3,4,6-tribromo- (4CI) (CA INDEX NAME)



RN 856356-94-0 CAPLUS  
CN 2,5-Acetoxyliide, 3,4,6-tribromo- (4CI) (CA INDEX NAME)



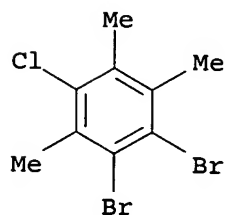
L11 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1936:13394 CAPLUS  
DOCUMENT NUMBER: 30:13394  
ORIGINAL REFERENCE NO.: 30:1751i,1752a-g  
TITLE: Polymethylenes. XV. The Jacobsen reaction 4  
AUTHOR(S): Smith, Lee I.; Moyle, Clarence L.  
SOURCE: Journal of the American Chemical Society (1936), 58, 1-10  
CODEN: JACSAT; ISSN: 0002-7863  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

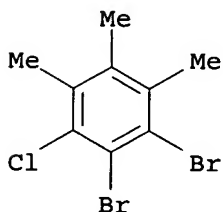
AB Chlorodurene, chloroisodurene and chloroprehnitene rearrange in contact with H<sub>2</sub>SO<sub>4</sub> to give chloropentamethyl-benzene (I) and 3-chloropseudocumene-5-sulfonic acid (II), a Me group migrating in such a manner that the same chlorotrimethylbenzene derivative resulted. Chloroisodurene also gives a small quantity of a compound, C<sub>20</sub>H<sub>24</sub>Cl<sub>2</sub>, m. 209.5°, the structure of which is not known. 5-Chloropseudocumene and the 6-isomer give II; chloromesitylene and 4-chlorohemimellitene were stable toward H<sub>2</sub>SO<sub>4</sub>. Bromomesitylene gives mesitylenesulfonic acid and di- or tribromomesitylene, depending upon the temperature; 5-bromopseudocumene gives largely 3-bromopseudo-cumene-5-sulfonic acid, together with a small quantity of tribromopseudocumene; no pseudocumene-5-sulfonic acid was found. The following did not rearrange with H<sub>2</sub>SO<sub>4</sub>: hemimellitene, 5-nitropseudocumene, 5-pseudocumidine, Me pentamethylbenzenesulfonate, pentamethyl-cyclohexane, 2,3-Cl<sub>10</sub>H<sub>6</sub>Me<sub>2</sub> and p-BrC<sub>6</sub>H<sub>4</sub>Ph. Yields are given, together with the conditions used. I was identified by analysis and conversion into C<sub>6</sub>HMe<sub>5</sub>; II was identified by conversion into the amide, m. 182°. 3-Chloro-5,6-dinitropseudocumene is reduced by SnCl<sub>2</sub> in

EtOH-HCl to the di-NH<sub>2</sub> derivative, m. 136.5°, stable in the air for some time; phenanthrenequinone (III) in AcOH-EtOH gives 12-chloro-10,11,13-trimethylphenanthrophenazine, yellow, m. 330.5-1°. Reduction of the di-NO<sub>2</sub> compound with SnCl<sub>2</sub> in AcOH-HCl yields 6-chloro-2,4,5,7-tetramethyl-benzimidazole, m. 250-1°. 5-Chloro-1,3-diaminomesitylene, m. 137-8°; this does not react with III or form a benzimidazole. Nitration of Na 4-chlorohemimellitene-sulfonate gives 4-chloro-5,6-dinitrohemimellitene, m. 182-2.5°; SnCl<sub>2</sub> in AcOH yields 7-chloro-2,4,5,6-tetramethyl-benzimidazole, m. 286.5-7.5°. 10,11,13-Trimethylphenanthrophenazine, yellow, m. 253°. Many other details are given of the preparation of products used for the identification of the compds. formed in the rearrangement, as well as starting materials. Na chloromesitylene-sulfonate crystallizes with 0.5 mol. H<sub>2</sub>O, as does the Br derivative; bromomesitylene-sulfonamide, m. 160-60.5°. 3-Chloro-5,6-dibromopseudocumene, m. 224°; 6-chloro-3,5-dinitro-pseudocumene, m. 162°. 6-Bromo-5-pseudocumidine, m. 69° (56.8% yield). 4-Chloro-5,6-dibromohemimellitene, m. 229-30°; 13-chloro-10,11,12-trimethylphenanthrophenazine, yellow, m. 346.5-7°. 7-Chloro-2,4,5,6-tetramethyl-benzimidazole, m. 288.5°. 10,11,12-Trimethylphenanthrophenazine, orange, m. 311°. Pentamethylbenzene-methanesulfonate, m. 91-1.5°. The ease of migration of groups present in the chloro- and bromotetramethyl-benzenes is in the order Br > Me > Cl; in case of the corresponding derivs. of the C<sub>6</sub>H<sub>3</sub>Me<sub>3</sub> the order is Br > Cl > Me. Attempts to find mild conditions which would cause Jacobsen rearrangements without producing amorphous by-products were unsuccessful. Dilution of the H<sub>2</sub>SO<sub>4</sub> with 10% of H<sub>2</sub>O or with H<sub>3</sub>PO<sub>4</sub> or AcOH inhibited the rearrangement and the side reaction as well. The use of CaCl<sub>2</sub>, Mg(ClO<sub>4</sub>)<sub>2</sub>, PhSO<sub>3</sub>H, AcOH or H<sub>3</sub>PO<sub>4</sub> merely caused hydrolysis of the sulfonic acid to the hydrocarbon and no reagents or conditions were found, other than those already known, which would cause any rearrangements to take place. Little can be said with regard to the mechanism of the reaction.

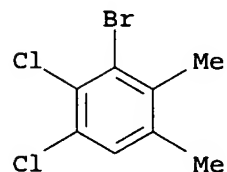
IT 856070-13-8, Pseudocumene, 5,6-dibromo-3-chloro-  
 859774-87-1, Hemimellitene, 4,5-dibromo-6-chloro-  
 (preparation of)  
 RN 856070-13-8 CAPLUS  
 CN Pseudocumene, 5,6-dibromo-3-chloro- (3CI) (CA INDEX NAME)



RN 859774-87-1 CAPLUS  
 CN Hemimellitene, 4,5-dibromo-6-chloro- (3CI) (CA INDEX NAME)



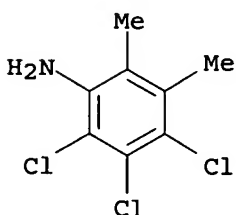
TITLE: Dichloro-o-xylene. II  
 AUTHOR(S): Hinkel, Leonard E.; Ayling, Ernest E.; Walters, Thomas M.  
 SOURCE: Journal of the Chemical Society (1934) 1946-8  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB cf. C. A. 22, 3638. 6-Chloro-o-3-xylidine through the Sandmeyer reaction gives 70% of 3,6-dichloro-o-xylene (I), b760 234° m. 29°; chlorination gives the 3,4,5,6-tetra-Cl derivative; nitration gives the 4-NO2 derivative (II), m. 84°; reduction with Fe and 5% AcOH gives 96% of 3,6-dichloro-o-4-xylidine, m. 54° (Ac derivative, m. 146°). The 4,5-di-NO2 derivative of I m. 174°; the 4,5-di-NH2 derivative m. 176° (phenazine derivative, m. above 250°). The 4,5-di-Br derivative of I m. 238°. 6-Chloro-4-nitro-o-3-xylidine through the Sandmeyer reaction gives II. 5-Chloro-o-4-xylidine gives 71% of 4,5-dichloro-o-xylene, m. 76°; 3,6-di-Br derivative, m. 232°; the 3-Br derivative, from 4,5-dichloro-o-3-xylidine, m. 111°. Chlorination of 3-chloro-o-xylene gives the 3,4-di-Cl derivative only; the 4-Cl derivative gives only the 4,5-di-Cl derivative Nitration of 4-chloro-o-xylene gives the 5-NO2 derivative, m. 63°, and a di-NO2 derivative, m. 111°.  
 IT 854861-53-3, o-Xylene, 3-bromo-4,5-dichloro- (preparation of)  
 RN 854861-53-3 CAPLUS  
 CN o-Xylene, 3-bromo-4,5-dichloro- (3CI) (CA INDEX NAME)



L11 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1934:28468 CAPLUS  
 DOCUMENT NUMBER: 28:28468  
 ORIGINAL REFERENCE NO.: 28:3389i,3390a-e  
 TITLE: Chlorination of the aceto-o-xylides  
 AUTHOR(S): Hinkel, Leonard E.; Ayling, Ernest E.; Walters, Thomas M.  
 SOURCE: Journal of the Chemical Society (1934) 283-7  
 CODEN: JCSOA9; ISSN: 0368-1769  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The extent of chlorination of aceto-o-3-xylide (I) depends mainly on the temperature; the yield of Cl derivs. varied with the strength of the AcOH used and was greatest (65%) in glacial AcOH at 10-12°; with dichloramine T the 4-Cl (II) and the 6-Cl derivative (III) were obtained in 17 and 65% yields, resp. II m. 169° and is difficult of isolation because of its ready solubility in organic solvents. With 2 mols. Cl in glacial AcOH above 40° I gives 4,6-dichloroaceto-o-3-xylide (IV), m. 188°; hydrolysis gives 4,6-dichloro-o-3-xylidine, m. 44°; at lower temps. some III was also formed; with excess Cl and an increase of temperature a mixture of IV and the 4,5,6-tri-Cl derivative was formed, which on hydrolysis gives 4,5,6-trichloro-o-3-xylidine, m. 207°. Chlorination of III in AcOH at 50° gives IV. III and HNO3 in AcOH, heated on a steam bath for 30 min., give 6-chloro-4-nitroaceto-o-3-xylide, m. 196.5°; hydrolysis with 40% H2SO4 gives 6-chloro-4-nitro-o-3-xylidine, m. 143°; reduction gives an o-diamine. I and KOCl give N-chloroaceto-o-3-xylide, m. 94.5°, readily transformed into a mixture of II and III. III yields a N,6-di-Cl derivative, m. 81°, transformed into IV. IV yields a N,4,6-tri-Cl derivative, isomerization of which regenerates IV. Chlorination of aceto-o-4-xylide (V) in AcOH with 1 mol. of Cl or with dichloramine T gives a mixture of the 5-Cl derivative (VI)

and the 3-Cl derivative (VII), m. 114°; hydrolysis of the latter gives 3-chloro-o-4-xylidine, m. 26°; both VI and VII are much less basic than II and III, their salts with HCl and H2SO4 being completely dissociated in dilute solution. The yield of VI and VII from V and dichloramine T in CHCl3 are 48 and 19%, resp., 22% V being recovered. N-Chloroaceto-o-4-xylide, m. 55°; warming in CHCl3 or AcOH gives 50% of VI and VII and 25% V. The N,5-di-Cl derivative m. 74° (90% yield); it is slowly transformed into the 3,5-di-Cl derivative in CHCl3 or AcOH at room temperature; warming in AcOH containing a little H2SO4 for 2 days gives 48% of the 3,5-di-Cl derivative and 10% of the 5-Cl derivative 3-Nitro-o-4-xylidine through the diazo reaction gives 60% of 4-chloro-3-nitro-o-xylene, pale yellow, m. 75°; reduction and acetylation gives II. The structure of IV follows from the removal of the NH2 groups from the free base, yielding 3,5-dichloro-o-xylene. 5-Chloro-4-nitro-o-xylene, pale yellow, m. 63°; reduction and acetylation gives VI; VII was synthesized from 4-nitro-o-3-xylidine.

IT 854857-43-5, 2,3-Xylidine, 4,5,6-trichloro-  
(preparation of)  
RN 854857-43-5 CAPLUS  
CN 2,3-Xylidine, 4,5,6-trichloro- (3CI) (CA INDEX NAME)



L11 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1930:53093 CAPLUS

DOCUMENT NUMBER: 24:53093

ORIGINAL REFERENCE NO.: 24:5731i,5732a-b

TITLE: The nitration of 5-bromo-1,3-dimethyl-4-acetamidobenzene and 3,5-dibromo-1,4-dimethyl-2-acetamidobenzene and some derivatives

AUTHOR(S): Bures, E.; Smetana, J.

SOURCE: Casopis Ceskoslovenskeho Lekarnictva (1930),  
10, 99-102,131-7,160-4

CODEN: CCLEA3

DOCUMENT TYPE: Journal

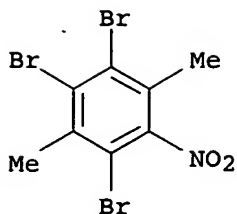
LANGUAGE: Unavailable

AB 6,2,4-BrMe2C6H2NH2, m. 49-50°, wits converted into its Ac derivative m. 197-8°, which on nitration gave 5-bromo-2,6-dinitro-1,3-dimethyl-4-acetamidobenzene, m. 278°, from which were prepared:  
5-bromo-2,6-dinitro-1,3-dimethyl-4-aminobenzen, m. 171-2°;  
5-bromo-2,6-dinitro 1,3-dimethylbenzene, m. 67°;  
4,5-dibromo-2,6-dinitro-1,3-dimethylbenzene, m. 193°. From p-xylidinc were prepared 3,5-dibromo-1,4-dimethyl-2-aminobenzene, m. 65°. and its Ac derivative, m. 193°. Nitration of 2,5,4,6-Me2Br2C5H2NHAc gave 3,5 dibromo-6-nitro-1,4-dimethyl-2-acetamidobenzene, m. 264-.5 °, from which were prepared:  
3,5-dibromo-6-nitro-1,4-dimethyl-2-aminobenzene, m. 176°;  
3,5-dibromo-6-nitro-1,4 dimethylbenzene, m. 69°;  
2,3,5-tribromo-6-nitro-1,4-dimethylbenzene, m. 207°; 3,5-dibromo-2-iodo-6-nitro-1,4-dimethylbenzene, m. 204°.

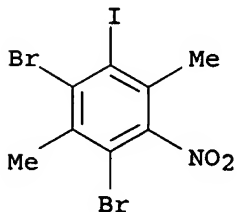
IT 854861-22-6, p-Xylene, 2,3,5-tribromo-6-nitro- 854861-35-1  
, p-Xylene, 2,6-dibromo-3-iodo-5-nitro-  
(preparation of)

RN 854861-22-6 CAPLUS

CN p-Xylene, 2,3,5-tribromo-6-nitro- (3CI) (CA INDEX NAME)



RN 854861-35-1 CAPLUS  
 CN p-Xylene, 2,6-dibromo-3-iodo-5-nitro- (3CI) (CA INDEX NAME)



L11 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

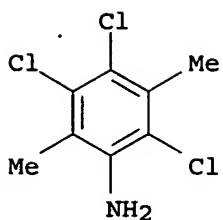
ACCESSION NUMBER: 1930:16898 CAPLUS  
 DOCUMENT NUMBER: 24:16898  
 ORIGINAL REFERENCE NO.: 24:1851b-d  
 TITLE: 1,4-Dimethyl-3,5,6-trichloro-2-aminobenzene and some of its derivatives  
 AUTHOR(S): Bures, E.; Rubes, T.  
 SOURCE: Collection of Czechoslovak Chemical Communications (1929), 1, 648-57  
 CODEN: CCCCAK; ISSN: 0010-0765  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB 1,4-Dimethyl-2-acetamidobenzene in a large excess of anhydrous AcOH gives quantitatively 1,4-dimethyl-3,5,6-trichloro-2-acetamidobenzene (I), m. 222°, by direct chlorination. Saponification of I gives quant. the 2-amino compound (II), m. 206°, whose Bz derivative m. 223°. II and Me2SO4 give the 2-methylamino derivative, m. 62°. The picrate of II, red-purple crystals, m. above 100° (decomposition) and is decomposed into its constituents by H2O. By diazotization of II, 1,4-dimethyl-3,5,6-trichloro-2-hydroxybenzene (III), m. 175°, is obtained: its alkaline solution treated with Me2SO4 gives the corresponding MeO derivative, m. 91°, while Et2SO4 gives the EtO derivative, m. 79°. The benzoate of III m. 101°, and the acetate m. 103°. A solution of the Na salt of III, treated with HgCl2, ppts. a basic Hg salt containing 28.22% Hg. A basic Bi salt can be similarly obtained. 1,4-Dimethyl-3,5,6-trichlorobenzene, m. 96°, is obtained from II by diazotization; 1,4-dimethyl-2,3,5,6-tetrachlorobenzene, m. 223°, is similarly obtained from II; 1,4-dimethyl-3,5,6-trichloro-2-cyanobenzene, m. 213°, is also similarly obtained.

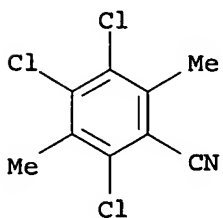
IT 857974-28-8, 2,5-Xylidine, 3,4,6-trichloro- 859202-54-3, Isoxylonitrile, 3,4,6-trichloro- 872275-60-0, 2,5-Xylidine, 3,4,6-trichloro-N-methyl- 873979-22-7, 2,5-Acetoxylide, 3,4,6-trichloro- 873987-55-4, 2,5-Benzoxylide, 3',4',6'-trichloro- 876486-92-9, Phenetole, 2,4,5-trichloro-3,6-dimethyl- (preparation of)

RN 857974-28-8 CAPLUS  
 CN 2,5-Xylidine, 3,4,6-trichloro- (5CI) (CA INDEX NAME)

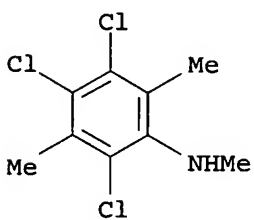




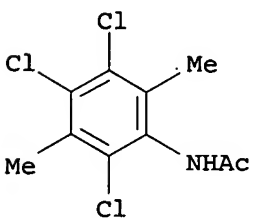
RN 859202-54-3 CAPLUS  
 CN 2,5-Xylonitrile, 3,4,6-trichloro- (3CI) (CA INDEX NAME)



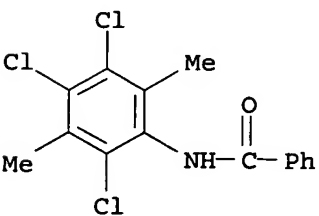
RN 872275-60-0 CAPLUS  
 CN 2,5-Xylidine, 3,4,6-trichloro-N-methyl- (3CI) (CA INDEX NAME)



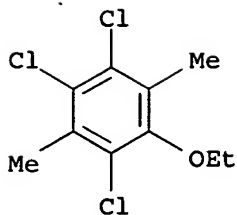
RN 873979-22-7 CAPLUS  
 CN 2,5-Acetoxyide, 3,4,6-trichloro- (3CI) (CA INDEX NAME)



RN 873987-55-4 CAPLUS  
 CN 2,5-Benzoxylide, 3',4',6'-trichloro- (3CI) (CA INDEX NAME)



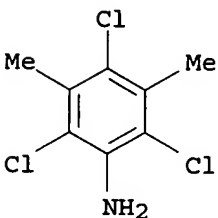
RN 876486-92-9 CAPLUS  
 CN INDEX NAME NOT YET ASSIGNED



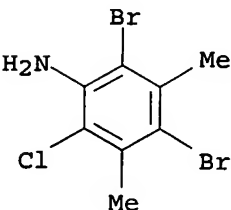
L11 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1930:6485 CAPLUS  
 DOCUMENT NUMBER: 24:6485  
 ORIGINAL REFERENCE NO.: 24:729i,730a-b  
 TITLE: Azo dyes  
 PATENT ASSIGNEE(S): I. G. Farbenindustrie AG  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	FR 663683		19290823	FR	19281108 <--
AB	<p>Azo dyes are prepared by combining the diazo compds. of halogen substitution products of 3,5-xylylidine with arylamides of compds. capable of coupling and possessing affinity for vegetable fibers, such as arylamides of 3-hydroxy-2-naphthoic acid, or the <math>\beta</math>-ketocarboxylic acids. Several examples and a table of components with the colors obtained are given. The following new derivs. of 3,5-xylylidine are given: 4-chloro-, m. 58-59°, 4-bromo-, m. 66-67°, 2-bromo-, m. 27-28°, b. 261-263°, 2,4-dichloro-, m. 71-72°, 2,6-dichloro-, m. 88-90°, 2,4,6-trichloro-, m. 188-189°, 4-bromo-2-chloro-, m. 70-72°, 4-chloro-2-bromo-, m. 79-80°, 2, 4-dibromo-, m. 81-82°, 2,4-dibromo-6-chloro-, m. 184-186°.</p>				
IT	854854-81-2, 3,5-Xylylidine, 2,4,6-trichloro- 854854-86-7, 3,5-Xylylidine, 2,4-dibromo-6-chloro- (preparation of)				
RN	854854-81-2 CAPLUS				
CN	3,5-Xylylidine, 2,4,6-trichloro- (3CI) (CA INDEX NAME)				



RN 854854-86-7 CAPLUS  
 CN 3,5-Xylylidine, 2,4-dibromo-6-chloro- (3CI) (CA INDEX NAME)



ACCESSION NUMBER: 1929:31223 CAPLUS  
 DOCUMENT NUMBER: 23:31223  
 ORIGINAL REFERENCE NO.: 23:3674g-i  
 TITLE: 1,4-Dimethyl-3,5,6-trichloro-2-aminobenzene and some  
 of its derivatives  
 AUTHOR(S): Bures, E.; Rubes, T.  
 SOURCE: Casopis Ceskoslovenskeho Lekarnictva (1928),  
 8, 225-31,258-64  
 CODEN: CCLEA3  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

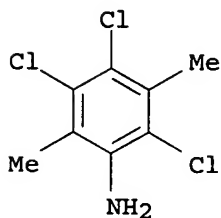
AB By the action of Cl<sub>2</sub> on 2,5-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>NHAc in glacial AcOH at ordinary temperature  
 and pressure, without catalyst. B. and R. obtained 1,4-dimethyl-3,5,6-  
 trichloro-2-acetamidobenzene m. 222°, which on hydrolysis gave the  
 2-amino compound, m. 206° (I). From I were prepared the Bz derivative, m.  
 223°, the picrate, m. above 100° (decomposition), and the  
 2-methylamino compound, m. 62°. There were also prepared  
 1,4-dimethyl-1-3,5,6-trichloro-2-hydroxybenzene, m. 175° (Me ether,  
 m. 91°; Et ether, m. 79°; benzoate, m. 101°; acetate,  
 m. 103°) 1,4-dimethyl-3,5,6-trichlorobenzene, m. 96°;  
 1,4-dimethyl-2,3,5,6-tetrachlorobenzene, m. 223°;  
 1,4-dimethyl-3,5,6-trichloro-2-benzonitrile, m. 213°.

IT 857974-28-8, 2,5-Xylidine, 3,4,6-trichloro- 859202-54-3,  
 2,5-Xylonitrile, 3,4,6-trichloro- 872275-60-0, 2,5-Xylidine,  
 3,4,6-trichloro-N-methyl- 873979-22-7, 2,5-Acetoxylyde,  
 3,4,6-trichloro- 873987-55-4, 2,5-Benzoxylide,  
 3',4',6'-trichloro- 876486-92-9, Phenetole, 2,4,5-trichloro-3,6-  
 dimethyl-

(preparation of)

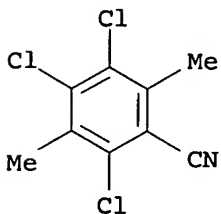
RN 857974-28-8 CAPLUS

CN 2,5-Xylidine, 3,4,6-trichloro- (5CI) (CA INDEX NAME)



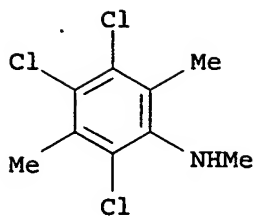
RN 859202-54-3 CAPLUS

CN 2,5-Xylonitrile, 3,4,6-trichloro- (3CI) (CA INDEX NAME)

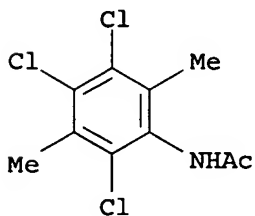


RN 872275-60-0 CAPLUS

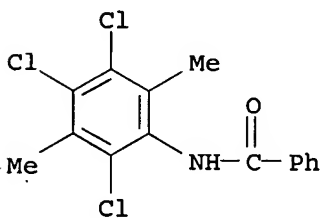
CN 2,5-Xylidine, 3,4,6-trichloro-N-methyl- (3CI) (CA INDEX NAME)



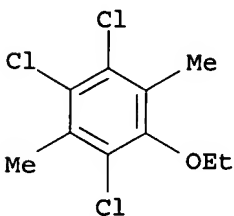
RN 873979-22-7 CAPLUS  
CN 2,5-Acetoxyldide, 3,4,6-trichloro- (3CI) (CA INDEX NAME)



RN 873987-55-4 CAPLUS  
CN 2,5-Benzoxylide, 3',4',6'-trichloro- (3CI) (CA INDEX NAME)



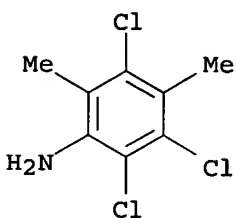
RN 876486-92-9 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED



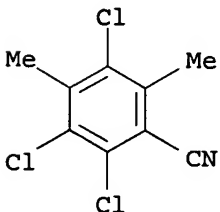
L11 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1928:37668 CAPLUS  
DOCUMENT NUMBER: 22:37668  
ORIGINAL REFERENCE NO.: 22:4503h-i,4504a  
TITLE: 2,5,6-Trichloro-1,3-dimethyl-4-aminobenzene and some  
of its derivatives  
AUTHOR(S): Bures, E.; Borgmann, J.  
CORPORATE SOURCE: Charles Univ., Prague  
SOURCE: Casopis Ceskoslovenskeho Lekarnictva (1927),  
7, 270-80  
CODEN: CCLEA3  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB By the action of Cl on 2,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>NHAc, m. 123°, dissolved in  
glacial AcOH, at ordinary temperature and pressure, without catalysts, is formed  
2,5,6-trichloro-1,3-dimethyl-4-acetamidobenzene, m. 208.5° (I).

The introduction of the 3 Cl atoms stabilizes the mol. and lowers the basicity of the amine. I on saponification yields 2,5,6-trichloro-1,3-dimethyl-4-aminobenzene, m. 204° (II) (Bz derivative, m. 174-5°; HCl salt, m. 217°). II was converted to 2,5,6-trichloro-1,3-dimethyl-4-hydroxybenzene, m. 174° (Me ether, m. 91.5°; Et ether, m. 53.5°; Ac ester, m. 86°). Other derivs. of II prepared were 2,5,6-trichloro-1,3-dimethylbenzene, m. 179.5°; 2,5,6-trichloro-1,3-dimethyl-4-benzonitrile, m. 218°, which on hydrolysis gave 3,5,6-trichloro-2,4-dimethylbenzoic acid, m. 191.5°; and 2,4,5,6-tetrachloro-1,3-dimethylbenzene, m. 219°.

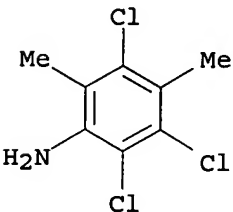
IT 854824-50-3, 2,4-Xylidine, 3,5,6-trichloro- 854854-59-4,  
2,4-Xylonitrile, 3,5,6-trichloro- 854857-20-8, 2,4-Xylidine,  
3,5,6-trichloro-, -HCl 854857-71-9, 2,4-Xylic acid,  
3,5,6-trichloro- 854858-61-0, 2,4-Xylenol, 3,5,6-trichloro-,  
acetate 860567-17-5, 2,4-Benzoxylide, 3',5',6'-trichloro-  
860580-56-9, 2,4-Acetoxylyde, 3,5,6-trichloro-  
(preparation of)  
RN 854824-50-3 CAPLUS  
CN 2,4-Xylidine, 3,5,6-trichloro- (3CI) (CA INDEX NAME)



RN 854854-59-4 CAPLUS  
CN 2,4-Xylonitrile, 3,5,6-trichloro- (3CI) (CA INDEX NAME)

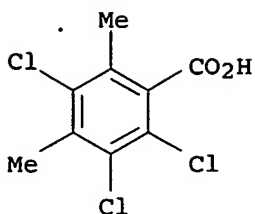


RN 854857-20-8 CAPLUS  
CN 2,4-Xylidine, 3,5,6-trichloro-, -HCl (3CI) (CA INDEX NAME)

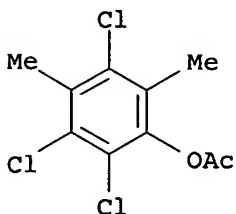


● HCl

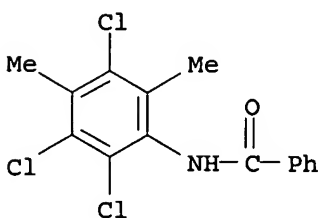
RN 854857-71-9 CAPLUS  
CN 2,4-Xylic acid, 3,5,6-trichloro- (3CI) (CA INDEX NAME)



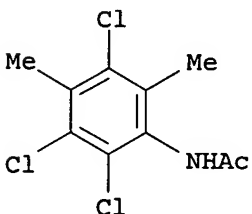
RN 854858-61-0 CAPLUS  
 CN 2,4-Xylenol, 3,5,6-trichloro-, acetate (3CI) (CA INDEX NAME)



RN 860567-17-5 CAPLUS  
 CN 2,4-Benzoxylide, 3',5',6'-trichloro- (3CI) (CA INDEX NAME)



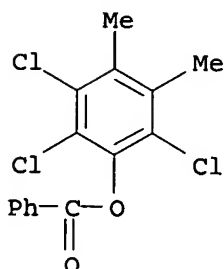
RN 860580-56-9 CAPLUS  
 CN 2,4-Acetoxylylde, 3,5,6-trichloro- (3CI) (CA INDEX NAME)



L11 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1925:1897 CAPLUS  
 DOCUMENT NUMBER: 19:1897  
 ORIGINAL REFERENCE NO.: 19:267g-i,268a  
 TITLE: Conversion of hydroaromatic into aromatic compounds.  
 I. Action of chlorine on 5-chloro-1,1-dimethyl-  
 Δ4-cyclohexen-3-one  
 AUTHOR(S): Hinkel, L. E.  
 SOURCE: Journal of the Chemical Society, Transactions (1924), 125, 1847-55  
 CODEN: JCHTA3; ISSN: 0368-1645  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB The finding that there is a divergence between the action of Cl and Br upon the same hydroaromatic compound, the former producing the more deep-seated change (C. A. 15, 56), is supported by the results of the

action of Cl on 5-chloro-1,1-dimethyl- $\Delta$ 4-cyclohexen-3-one (I), which is more profound than that of Br on the corresponding Br compound (C. A. 8, 1265). Cl passed rapidly into 40 g. I in its own volume of  $\text{CHCl}_3$  until the evolution of HCl almost ceased and the liquid regained normal temperature, gave the 3,4,5-Cl<sub>3</sub> derivative (II), m. 61°, boils with gradual decomposition, evolving HCl; alc. KOH gives 4-chloro-3,5-dihydroxy-0-xylene, m. 123° (di-Bz derivative, m. 137°); heated with  $\text{H}_2\text{SO}_4$  on the  $\text{H}_2\text{O}$  bath and finally at 110-20°, it gives 5,6-dichloro-0-4-xylene, m. 102° (Bz derivative, m. 94°); heated with  $\text{C}_9\text{H}_7\text{N}$  for 30 mins. at 170°, there results 4,5-dichloro-0-3-xylene, m. 95° (Bz derivative, m. 128°), which yields a tri-Cl derivative (III), m. 182.5° (Bz derivative, m. 120°) with Cl in light petroleum. II reacts with  $\text{C}_9\text{H}_7\text{N}$  to give 4,5-dichloro-0-3-xylene, m. 95° (Bz derivative, m. 128°), and with Cl yields a tetra-Cl derivative, m. 127.5°. If the reaction between I and Cl is carried out in well cooled  $\text{CHCl}_3$  there results a 4,5-di-Cl derivative, b.p. 120-1°, having a camphoraceous odor. Action of Cl at room temperature gave II; heating gives 5,3-Cl(HO) $\text{C}_6\text{H}_2\text{Me}_2$ , also obtained with alc. KOH.  $\text{H}_2\text{SO}_4$  gives 6-chloro-0-3-xylene (IV), m. 98° (Bz derivative, m. 182.5°), which was synthesized from 6-chloro-4-nitro-0-xylene, slightly yellow needles, m. 101°, through 6-chloro-0-4-xylidine, m. 72°. Cl and IV in  $\text{CHCl}_3$  give III. The filtrate from II gave some II and a fraction b.p. 145-55°, from which a 2,4,5,6-tetra-Cl derivative of I, m. 91°, crystallized; alc. KOH gave a di-Cl xylene, m. 119-20° (Bz derivative, m. 129°).  $\text{H}_2\text{SO}_4$  yielded a mixture of tri-chloro-o-3- and 4-xylene.

IT 861555-82-0, 3,4-Xylenol, 2,5,6-trichloro-, benzoate  
(preparation of)  
RN 861555-82-0 CAPLUS  
CN 3,4-Xylenol, 2,5,6-trichloro-, benzoate (2CI) (CA INDEX NAME)



L11 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1921:340 CAPLUS

DOCUMENT NUMBER: 15:340

ORIGINAL REFERENCE NO.: 15:56e-i

TITLE: Action of chlorine on 3,5-dichloro-1,1-dimethyl- $\Delta$ 2,4-cyclohexadiene

AUTHOR(S): Hinkel, Leonard E.

SOURCE: Journal of the Chemical Society, Transactions (1920), 117, 1296-1303

CODEN: JCHTA3; ISSN: 0368-1645

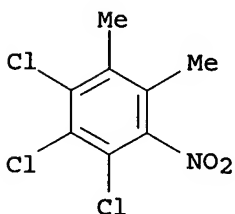
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

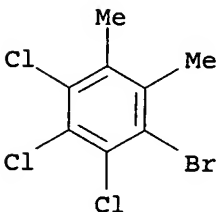
AB The action of Br (1 and 2 mols.) on 3,5-dichloro-1,1-dimethyl- $\Delta$ 2,4-cyclohexadiene (A) has been investigated by Crossley (J. Chemical Society 85, 264(1904)) and the action of Cl on A was studied to throw more light on the mechanism of the reaction. When A in dry  $\text{CHCl}_3$  is treated with Cl, HCl is evolved and after removal of the solvent the yellow product deposited in vacuo over NaOH in colorless prisms, m. 103.5°, is 2,3,3,4,5-pentachloro-1,1-dimethyl- $\Delta$ 5-cyclohexene (B), soluble in  $\text{Et}_2\text{O}$ ,  $\text{CHCl}_3$ ,  $\text{Me}_2\text{CO}$ ,  $\text{C}_6\text{H}_6$ . When B is heated at 120-30° HCl is evolved and on cooling crystals of 1,2,3,4,5- $\text{C}_6\text{HMe}_2\text{Cl}_3$  (C) separated (Ber. 18, 1369(1885)). B interacted vigorously with fuming  $\text{HNO}_3$  and the product treated with  $\text{H}_2\text{O}$ , washed and crystallized from  $\text{AcOEt}$ , m. 223-4°, and is 3,4,5,6-Cl<sub>4</sub> $\text{C}_6\text{Me}_2$  (D). The mother liquors from which B separated gave off HCl

when heated to 180-200°, and when distilled gave 3,5,6-trichloro-o-xylene (E), m. 47.5°, and also C and D. When C was treated in dry CHCl<sub>3</sub> with Fe and Cl, D resulted and with Br gave needles, m. 226°, of 3,4,5-trichloro-6-bromo-o-xylene (F), readily soluble in Et<sub>2</sub>O, C<sub>6</sub>H<sub>6</sub>, and sparingly soluble in CHCl<sub>3</sub> and alc. When C is treated with fuming HNO<sub>3</sub> and the product is washed with H<sub>2</sub>O and crystallized from alc. stout yellowish needles, m. 149°, of 3,4,5-trichloro-6-nitro-o-xylene (G) are formed. This product is soluble in Et<sub>2</sub>O, C<sub>6</sub>H<sub>6</sub>, CHCl<sub>3</sub> and light petroleum. C was prepared from o-4-xylidene (Crossley, loc. cit.) by acetylating, chlorinating and treating in HCl with CuCl and NaNO<sub>2</sub>. When A in cold CHCl<sub>3</sub> was treated with Cl, no crystalline product could be secured and on distilling the liquid, 3 fractions (1) 217-20°, (2) 222-6°, and (3) 228-33°, were obtained. Fraction 2 gave a product which on treatment with Br and Fe gave 3,5,4,6-Cl<sub>2</sub>Br<sub>2</sub>C<sub>6</sub>Me<sub>2</sub> (H) (loc. cit.) and fraction 3 contained E. When E was treated in CHCl<sub>3</sub> with Br and Fe, H was formed, and when treated with fuming HNO<sub>3</sub> the resulting product was 3,5,4,6-Cl<sub>2</sub>(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>Me<sub>2</sub>.

IT 861555-92-2, o-Xylene, 3,4,5-trichloro-6-nitro-  
 861614-30-4, o-Xylene, 3-bromo-4,5,6-trichloro-  
 (preparation of)  
 RN 861555-92-2 CAPLUS  
 CN o-Xylene, 3,4,5-trichloro-6-nitro- (2CI) (CA INDEX NAME)



RN 861614-30-4 CAPLUS  
 CN o-Xylene, 3-bromo-4,5,6-trichloro- (2CI) (CA INDEX NAME)



L11 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

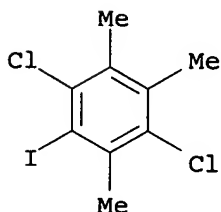
ACCESSION NUMBER: 1912:5489 CAPLUS  
 DOCUMENT NUMBER: 6:5489  
 ORIGINAL REFERENCE NO.: 6:859f-i,860a  
 TITLE: s-Iodopseudocumene and Derivatives  
 AUTHOR(S): Willgerodt, C.; Meyer, R.  
 CORPORATE SOURCE: Univ. Freiburg  
 SOURCE: Ann. (1912), 385, 341-51  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB s-Iodopseudocumene, prepared by dissolving 11 g. pseudocumene in 100 cc. petroleum ether and b. with 20 g. sulfur iodide in 100 cc. HNO<sub>3</sub> (1.34) 4 hrs. on the water bath. M. 37°. s-Pseudocumyliodide chloride, C<sub>9</sub>H<sub>11</sub>Cl<sub>2</sub>I, yellow crystals, decompose, 66°. s-Iodosopseudocumene, C<sub>9</sub>H<sub>11</sub>OI, yellowish white powder, decompose, 171°. Acetate, needles, m. 123°. s-Iodopseudocumene, C<sub>9</sub>H<sub>11</sub>O<sub>3</sub>I, jelly-like, explodes about 210°. Di-s-pseudocumyliodinium; compounds. Hydroxide, could not be obtained pure. Hydrochloride, crystalline powder, m. 107°. Chloroplatinate, crystalline powder, m. 159°. Chloroaurate, needles from alc., m. 90°. Hydrobromide needles from alc., m. 118°.



Hydriodide, m. 120°. Dichromate, amorphous precipitate, explodes at 120°. Monoiodo-di-s-pseudocumyliodinium compds. Anion = C9H(C9H10I). Hydrochloride, m. 106°. Chloroplatinate, m. 150°. Chloromercurate, amorphous, m. 108°. Chloroaurate, amorphous, Hydrobromide, bright yellow amorphous mass, m. 105°. Hydriodide, amorphous powder, m. 112°. Dichromate, decamp. 113°. Phenyl-s-pseudocumyliodinium compds. Anion = PhC9H11I. Hydrochloride, crystalline powder, m. 186°. Chloroplatinate, amorphous, m. 188°. Chloroaurate, crystalline precipitate, m. 117°. Chloromercurate, needles from alc., m. 161°. Hydrobromide, needles from H2O, m. 173°. Hydriodide, crystalline, decompose 147°. Dichromate, crystalline powder, explodes at 184°. p-Tolyl-s-pseudocumyliodinium compds. Anion = C7H7(C9H11)I. Hydrochloride, needles from H2O, m. 171°. Chloroplatinate, leaves from alc., decompose about 165°. Chloroaurate, needles, m. 71°. Chloromercurate, needles, m. 81°. Hydrobromide, crystalline powder, m. 148°. Hydriodide, decompose 108°. Dichromate, needles, decompose 149°. Dichlorobinyl-s-pseudocumyliodinium compds. Anion = CHCl = CCl(C9H11)I. Hydrochloride, m. 169°. Chloroplatinate, crystalline powder, decompose 150°. Chloroaurate, crystalline, m. about 134°. Hydrobromide, amorphous, m. 131°. Hydriodide, amorphous, m. 96°. p-Dichloro-s-iodopseudocumene, C9H9Cl2I, beautiful crystals from C6H6 m. 188-9°. Attempts to prepare the iodide chloride failed.

IT 859954-77-1, Pseudocumene, 3,6-dichloro-5-iodo-  
(preparation of)  
RN 859954-77-1 CAPLUS  
CN Pseudocumene, 3,6-dichloro-5-iodo- (1CI) (CA INDEX NAME)



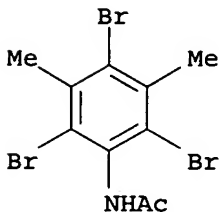
L11 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1910:4457 CAPLUS  
DOCUMENT NUMBER: 4:4457  
ORIGINAL REFERENCE NO.: 4:752d-h  
TITLE: Acetylation with Acetic Anhydride and Sulphuric Acid  
AUTHOR(S): Blanksma, J. J.  
SOURCE: Amsterdam. Chem. Weekblad (1910), 6, 717-27  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB By addition of a drop of concentrate H2SO4 to the reaction mixture, the acetylation of PhNH2 and its OH derivative is greatly accelerated, the following Ac2 derivs. being thus prepared, some, within a few min.:  
Di-acetyl-o-nitroaniline, colorless crystals, m. 94°. 2,4,6-Trinitro-m-diacetophenylene-diamine, colorless crystals, decompose 300°. 2,4,6-Tribromo-m-acetotoluide, colorless crystals, m. 205°, and the diacetyl derivative, colorless crystals, m. 103°. The former, with HNO3, yields 2,4,6,tribromo-5-nitro-m-acetotoluide, colorless needles, m. 261°, which, heated with concentrate H2SO4, gives 2,4,6-tribromo-5-nitro-m-toluidine, light yellow needles, m. 184°. Diacetyl derivative, colorless crystals, m. 188°. 2,4,6-Tribromo-sym-acetoxylidide, colorless crystals, m. 258°. 2,4,6-Tribromo-3,5-acetonitroaniline, colorless needles, m. 275°, which, by boiling with Ac2O and H2SO4, gives the diacetyl derivative, m. 165°. From 4-nitro-o-toluidine, with AcOH and Br., 3,5-dibromo-4-nitro-o-toluidine, yellow crystals, m. 104°. Acetyl derivatives, colorless crystals, m. 201°. Diacetyl derivative, m. 159°. The monoacetyl derivative, with HNO3 and H2SO4, gives 4,6-dinitro-3,5-dibromoacetotoluide, m. 280°. Similarly,

- 3,5-dibromo-2-nitro-ptoluidine, yellow crystals, m. 82°, and
- 2,6-dinitro-3,5-dibromo-p-acetotoluide, colorless crystals, m. 275° (KUNCKELL, 267°), which, with concentrate H<sub>2</sub>SO<sub>4</sub>, gives, 2,4-dinitro-3,5-dibromo-p-toluidine, dark yellow needles, m. 174°. Of the substituted phenol derivs. were prepared 2,4-dinitrophenyl acetate, colorless crystals, m. 72°, and 2,4-dibromo-6-nitrophenyl acetate, colorless crystals, m. 88°. Similarly, 8-methylfurfurylidene diacetate, large colorless, transparent crystals, m. 25°, and triacetyl β-hydroxy-8-methylfurfuraldehyde, colorless, transparent crystals, from ligroin, m. 73°.

IT 861611-09-8, 3,5-Acetoxyliide, 2,4,6-tribromo-  
 (preparation of)  
 RN 861611-09-8 CAPLUS  
 CN 3,5-Acetoxyliide, 2,4,6-tribromo- (1CI) (CA INDEX NAME)

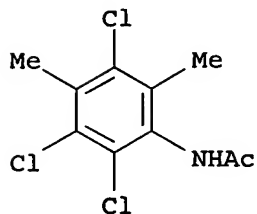


L11 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN

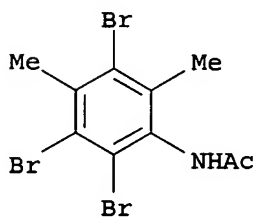
ACCESSION NUMBER: 1908:13564 CAPLUS  
 DOCUMENT NUMBER: 2:13564  
 ORIGINAL REFERENCE NO.: 2:2952g-i,2953a-b  
 TITLE: Preparation of Halogen-Substituted Anilides  
 AUTHOR(S): Mannino, A.; Didonato, L.  
 CORPORATE SOURCE: Ist. chim. R. Univ. Roma  
 SOURCE: Gazzetta Chimica Italiana (1908), 38(2), 20-31  
 CODEN: GCITA9; ISSN: 0016-5603  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable

AB A systematic study of the action of mixtures of concentrate HCl + HNO<sub>3</sub> and of HBr + HNO<sub>3</sub> upon acetanilide and its homologues confirms and extends the observations of Schloss (Diss. Lausanne 1901) and of Verda (Gazz. chim. ital., 32, [2], 20). In each case a single halo-gen-substituted amide is produced, without by-products and without the elimination of acetyl. Acetanilide with HCl and HNO<sub>3</sub> produces, on heating, 2,4-dichloracetanilide, but, if the reaction is carried on farther, all is converted into 2,4,6-trichloracetanilide; the latter is also obtained starting with o- or p-chloracetanilide, while m-chloracetanilide yields 3,5-dichloracetanilide. The HBr mixture produces with the same substances, in the above order, 2,4-dibromacetanilide, 2-chlor-4-bromacetanilide, 4-chlor-2-bromacetanilide, and a 3-chlor-2(?) -bromacetanilide, m. 105-7°. From m-bromacetanilide with the HCl mixture there result brilliant flesh-colored needles, m. 194-5°, which are probably 4,6-dichlor-3-bromacetanilide; with the HBr mixture, 2,4,5-tribromacetanilide, white needles, m. 188-9°. Paranitracetanilide yields 2-chlor-4-nitro-acetanilide, and an unidentified bromine compound. Acetyl-o-toluidine yields dichloracetyl-o-toluidine and 5-brom-acetyl-2-toluidine as shown by Verda, but the p-compound takes up 3 Cl or 2 Br. Acetyl-m-xylylidine yields trichloracetylmetaxylidine, white needles, m. 190-2°, and tribromacetylmetaxylidine, m. 246-8°. Acetyl-α-naphthylamine, with aqua regia takes up 1 Cl and 1 NO, as already observed by Verda. Saponification with 15% HCl produces a chloronitro-α-naphthylamine, yellow needles, m. 230°; with the HBr mixture, 3,8-dibrom-acetyl-α-naphthylamine is formed. Acetyl-β-naphthylamine yields a tribrominated substance, m. 250°, as also does 1,3,6-tribromacetyl-β-naphthylamine; but, on saponification, a base is formed, m. 125°, while the 1,3,6-tribrom-β-naphthylamine m. 143°, according to Claus and Philipson (J. pr.

Chemical [2], 43, 56).  
IT \* 860580-56-9, 2,4-Acetoxylylde, 3,5,6-trichloro- 861611-23-6  
, 2,4-Acetoxylylde, 3,5,6-tribromo-  
(preparation of)  
RN 860580-56-9 CAPLUS  
CN 2,4-Acetoxylylde, 3,5,6-trichloro- (3CI) (CA INDEX NAME)

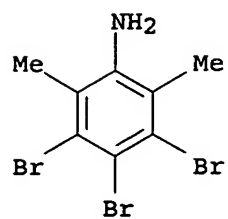


RN 861611-23-6 CAPLUS  
CN 2,4-Acetoxylylde, 3,5,6-tribromo- (1CI) (CA INDEX NAME)

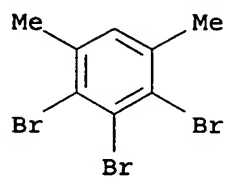


L11 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1907:1262 CAPLUS  
DOCUMENT NUMBER: 1:1262  
ORIGINAL REFERENCE NO.: 1:328i,329a-c  
TITLE: The Three Isomeric Tribromxylenes  
AUTHOR(S): Jaeger, F. M.; Blanksma, J. J.  
CORPORATE SOURCE: Univ. of Amsterdam  
SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la  
Belgique (1907), 25, 352-63  
CODEN: RTCPB4; ISSN: 0370-7539  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB A. Tribrom-o-xylenes. Bromination of the xylidines 1,2,3 and 1,2,4 gave  
4,6-dibrom-1,2,3-xylidine, m. 56°, and 3,5-dibrom-1,2,4-xylidine,  
m. 63°. Replacing the amino group in each by bromine yielded  
3,4,6-tribrom-o-xylene, m. 86, and 3,4,5-tribrom-o-xylene, m. 105°.  
Bromination of 1,2,4-acetxylidide gave 3,6-dibrom-1,2,4-xylidine, m.  
65°, which in turn gave the 3,4,6-tribrom-o-xylene. B.  
Tribrom-m-xylenes. The 2,4,6-tribrom-m-xylene, m. 85°, was  
obtained from 1,3,5-xylidine, 4,6-dibrom-2-aminoxylene 2-aminoxylene and  
1,3,4-acetxylidide. 2,4,6-Tribromxylidine, m. 195°.  
6-Brom-4-amino-m-xylene, m. 96°. 2-6-Dibrom-4-aminoxylene, m.  
65°. 4,5,6-Tribrom-m-xylene, m. 105°, came from  
4,6-dibrom-2-amino-m-xylene and 6-brom-4-amino-m-xylene.  
4,5,6-Dibrom-2-amino-m-xylene, m. 197°. 4,6-Dibrom-m-xylene, m.  
69°. 4,6-Dibrom-2,5-dinitro-m-xylene, m. 252°.  
4,5-Dibrom-m-xylene, b. 256°, m. 11°. 4,5-Dibrom-2,6-  
dinitroxylene, m. 193°. 2,6-Dibrom-4-amino-m-xylene, m.  
65°. 5,6-Dibrom-4-amino-m-xylene, m. 38°,  
2,4,5-Tribrom-m-xylene, m. 87°, was obtained from  
4-brom-2-amino-m-xylene. 4,5-Dibrom-2-amino-m-xylene, m. 51°. C.  
Tribrom-p-xylene, m. 89°, was obtained by bromination of  
1,4,5-xylidine, followed by replacement of the amino group by bromine.  
IT 860747-80-4, 2,6-Xylidine, 3,4,5-tribromo- 860748-31-8,  
m-Xylene, 4,5,6-tribromo- 860748-32-9, m-Xylene, 2,4,5-tribromo-  
(preparation of)

RN 860747-80-4 CAPLUS  
CN 2,6-Xylidine, 3,4,5-tribromo- (1CI) (CA INDEX NAME)



RN 860748-31-8 CAPLUS  
CN m-Xylene, 4,5,6-tribromo- (1CI) (CA INDEX NAME)



RN 860748-32-9 CAPLUS  
CN m-Xylene, 2,4,5-tribromo- (1CI) (CA INDEX NAME)

